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CITATION:

Saito, Keisuke ...[et al]. Influence of the Axial Ligand on the Cationic Properties of the Chlorophyll Pair in Photosystem II from Thermosynechococcus vulcanus.. Biophysical journal 2012, 102(11): 2634-2640

ISSUE DATE:

2012-06-06

URL:

http://hdl.handle.net/2433/157230

Influence of the axial ligand on the cationic properties of the chlorophyll pair in photosystem II from *Thermosynechococcus vulcanus*

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Abbreviations:

Chl*a*, chlorophyll *a*; D1-H198A with a water ligand, D1-H198 PSII structural model that possess water molecules near D1-198; D1-H198A without a water ligand, D1-H198 PSII structural model that possess no water axial ligand or additional water molecules; E_m, (midpoint) redox potential; OEC, oxygen-evolving cluster; $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$, positively charged P_{D1}/P_{D2} Chl*a* monomer; PSII, photosystem II; QM/MM approach, quantum chemical/molecular mechanical approach; *T. elongatus*, *Thermosynechococcus elongatus*;

Abstract

Influence of the axial ligand of P_{D1} chlorophyll (D1-His198) on the redox potentials (E_m) of monomer chlorophylls P_{D1} and P_{D2} and the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ charge ratio was investigated by theoretical calculations using the photosystem II (PSII) crystal structure of *Thermosynechococcus vulcanus* analyzed at 1.9-Å resolution. It was found that the $E_m(P_{D1})$ / $E_m(P_{D2})$ values and $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio remained unchanged upon D1-H198Q mutation. However, $E_m(P_{D1})$ was increased more than $E_m(P_{D2})$ in the D1-H198A mutant, resulting in a more even distribution of the positive charge over P_{D1}/P_{D2}. Introduction of a water molecule as an axial ligand resulted in equal E_m values and $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratios between the mutant and wild type, thus confirming the presence of the water ligand in the mutant.

Keywords: Photosystem II, chlorophyll, spin density distribution, electron transfer, redox potential, P680

INTRODUCTION

The reaction center of photosystem II (PSII) is composed of the D1/D2 hetrodimer, harboring the chlorophyll *a* (Chl*a*) pair P_{D1}/P_{D2}, the accessory Chl*a* Chl_{D1}/Chl_{D2}, two pheophytin *a* $Pheo_{D1}/Pheo_{D2}$, and two quinones as the redox active cofactors. P680, which absorbs light at a wavelength of 680 nm, is formed by excitonic coupling among the four Chl*a* and two Pheo cofactors (*1*). Excitation of P680 leads to the formation of the $Chl_{D1}^{\bullet+}$ $Pheo_{D1}^{\bullet-}$ state (*1-3*), followed by the $[P_{D1}/P_{D2}]^{\bullet+}$ $Pheo_{D1}^{\bullet-}$ state. The resulting $[P_{D1}/P_{D2}]^{\bullet+}$ state serves as an electron abstractor for the oxygen-evolving cluster (OEC). Thus, water oxidation is ultimately achieved by the high redox potential for one-electron oxidation (E_m) of P680. Following the initial charge separation in the reaction center of PSII, the positive charge is distributed over P_{D1}/P_{D2}. The $[P_{D1}^{\bullet+}\ P_{D2}]/[P_{D1}\ P_{D2}^{\bullet+}]$ ratio ($P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio) or corresponding spin density distribution was reported to be 82/18 from ENDOR studies of spinach PSII (*4*) or 80/20 from flash induced spectroscopic studies of *Synechocystis* PCC 6803 PSII (*5*), suggesting a preferential localization of the cationic state on P_{D1} over P_{D2} irrespective of the similarity in the protein sequences between D1 and D2 (*6*). The reason for the asymmetric distribution of the cationic state appears to be largely due to differences in several D1/D2 residue pairs, namely, D1-Asn181/D2-Arg180, D1-Asn298/D2-Arg294, D1-Asp61/D2-His61, D1-Glu189/D2-Phe188, and D1-Asp170/D2-Phe169 (*7*). These residues are conserved within the D1 or D2 protein family, respectively. Among these residues, those from the D1 side are either directly involved in the ligation of the Mn_4CaO_5-cluster or located in its vicinity, whereas in the D2 side, no such Mn_4CaO_5 cluster exists. Thus, these residues are either negatively charged or neutral in the D1 side, whereas their counterparts in the D2-side are largely positively charged or hydrophobic. This contributed significantly to the asymmetric distribution of the charge over the P_{D1}/P_{D2} pair (*7*).

In addition to the protein environment, axial ligands significantly influence the redox potential (E_m) of redox-active groups. In particular, the axial ligand replacement of heme proteins has been widely investigated using proteins and/or model systems. His ligands are likely to stabilize the oxidized state of heme, and thus lead to a decrease in E_m, i.e., the loss of a His axial ligand causes an increase in E_m (*8*). Similar behavior has been implied for chlorophylls in data obtained from computational studies (*9*). Mutations of the axial ligand of P_{D1}, D1-His198, would serve as a starting point from which to study the redox properties of P680. Surprisingly, mutations of D1-His198 to Ala had no effect on either the redox or spectroscopic properties of P680 in PSII from *Thermosynechococcus (T.) elongatus* (*10*). Although mutations of the axial ligands in PSII from *Synechocystis* PCC 6803 showed somewhat different properties, no obvious correlation between the spectral changes and the redox properties of P680 was found (*5*). It was proposed that the differences in the sequence of the D1 subunit in the two organisms might account for the detailed difference (*10*). However, the exact molecular geometry in the neighborhood of the P_{D1}/P_{D2} Chl*a* in *Synechocystis* PCC 6803 PSII remains unknown due to the lack of the crystal structure.

Since the *T. elongatus* PSII (*11; 12*) possesses a high degree of structural similarity to the *T. vulcanus* PSII (*13*), we investigated the influence of His ligand mutations with Gln and Ala on $E_m(P_{D1})$ and $E_m(P_{D2})$ using the *T. vulcanus* PSII crystal structure analyzed at a 1.9-Å resolution (*13*). The $E_m(P_{D1})$ and $E_m(P_{D2})$ values obtained represent those of monomeric Chl*a* and do not directly account for the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio for the Chl*a* pair. Thus, we also calculated the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio for the P_{D1}/P_{D2} Chl*a* pair using a large-scale quantum chemical/molecular mechanical (QM/MM) approach with the explicit treatment of the complete PSII atomic coordinates; defining the P_{D1}/P_{D2} pair as the QM region and the remaining protein subunits and cofactors as the MM region. Distributions of the positively charged state (*14; 15*) or spin density (*4; 5*) over the P_{D1}/P_{D2} chlorophyll pair have been measured in spectroscopic studies and can be compared with the present calculated results. Note that in general, electrostatic calculations and QM/MM calculations provide consistent results (*7; 16*).

METHODS

As demonstrated in the previous article (*7*), we employed the following systematic modeling procedure: First, we constructed a realistic molecular model of the whole PSII complex using the resent high-resolution crystal structure. On the basis of this atomistic model, we next evaluated the redox potential of P_{D1}/P_{D2} by solving the linear Poisson-Boltzmann equation with an explicit consideration of the protonation states for all titratable residues. Second, to obtain deeper insight into the electronic structure of P_{D1}/P_{D2} Chl*a* pair, we performed large-scale QM/MM calculations for the entire PSII complex. Finally, after confirming the validity of the present computational results through ~~the~~ comparison with available experimental data, we discussed the origin that determines the asymmetric distribution of the cationic state of P_{D1}/P_{D2} Chl*a* pair. Technical details of each modeling procedure are summarized as follows.

Coordinates. The atomic coordinates of PSII were taken from the X-ray structure of the PSII complexes from *T. vulcanus* at 1.9 Å resolution (PDB ID: 3ARC) (*13*). Hydrogen atoms were generated and energetically optimized with CHARMM (*17*), whereas the positions of all non-hydrogen atoms were fixed, and all titratable groups were kept in their standard protonation states, i.e., acidic groups were ionized and basic groups were protonated. For the QM/MM calculations, we added additional counter ions to neutralize the whole system.

Atomic partial charges. Atomic partial charges of the amino acids were adopted from the all-atom CHARMM22 (*18*) parameter set. The charges of the protonated acidic O atoms were increased symmetrically by +0.5 unit charges to implicitly account for the presence of a proton. Similarly, instead of removing a proton in the deprotonated state, the charges of all of the protons of the basic groups of Arg and Lys were diminished symmetrically by a total unit charge. For residues for which the protonation states were not available in the CHARMM22 parameter set, appropriate charges were computed (*19*). For the cofactors (e.g., the OEC cluster, Chl*a*, Pheo*a*, and quinones), the same atomic charges as in previous computations of PSII (*7*) were used.

OEC models. In the S_1-state, the valences of the 4 Mn atoms are most probably 2 Mn(III) and 2 Mn(IV) ions (e.g., Refs. (*20; 21*)). The exact valences of the individual Mn atoms are unclear; however, we found that changing the charge distribution of each Mn atom from the above distribution did not affect our calculation results significantly (*7*). The protonation states of the O atoms (and thus the net charge of the OEC atoms) in the OEC cluster remain unclear. Although O1, O2, and O3 are likely to be unprotonated O^{2-} based on observations of the OEC geometry, the protonation states of O4 linking Mn4 and Mn3 in the Mn_3CaO_4-cubane, and O5 in one of the corners of the cubane linking Mn4 and the cubane, necessitate more deep investigation as they might be O^{2-}, protonated OH^-, or even H_2O. Due to the uncertainty, we evaluated all possible combinations of the O4 and O5 protonation states and we tentatively used the $O4H^-$ $O5H^-$ model (see Ref. (*7*) for further details).

Except for a few examples (*22*), the spin coupling of the Mn ions has not been considered in a number of studies where the PSII protein environment was explicitly modeled (e.g., recent QM/MM studies on the S1-state model of OEC by Batista, Brudvig, and coworkers (*20*)). In particular, (i) our focus is not on the OEC cluster, (ii) the OEC cluster was included in the MM region (see below and (*7*)), and (iii) the atomic charges of OEC do not differ significantly among the different spin structures (*22*). Thus, the spin coupling was not considered in the present study.

QM/MM calculations. In all QM/MM calculations reported here, we employed the so-called electrostatic embedding QM/MM scheme. In all QM/MM calculations, we used the Qsite (*23*) program code. Electrostatic as well as steric effects created by complex PSII architecture were explicitly considered in all present calculations. Due to the large system size of PSII, the QM region was limited

to either the P_{D1}/P_{D2} Chl*a* pair or the pair and their axial ligands, while other protein units and all co-factors were approximated by the MM force field. Since we have optimized the atomic partial charges for the OEC cluster, Chl*a*, Pheo*a*, and quinones, the present QM/MM partition was accurate enough to describe the electronic structure of the $[P_{D1}/P_{D2}]^{\bullet+}$ Chl*a* pair. To reliably determine the cationic character of $[P_{D1}/P_{D2}]^{\bullet+}$ Chl*a* pair, we employed the unrestricted DFT method with the B3LYP functional and LACVP* basis sets. The detailed geometry of $[P_{D1}/P_{D2}]^{\bullet+}$ Chl*a* pair was refined by the constrained QM/MM optimizations; the surrounding protein environment was considered as the MM whose atomistic coordinates were exactly fixed with the original X-ray coordinates. After obtaining the stable geometry of QM fragment, we then determined the ESP charges for the cationic state of $[P_{D1}/P_{D2}]^{\bullet+}$ Chl*a* pair in the presence of the entire PSII atomic coordinates (Tables S1 and S2, Supporting Information).

The potential-energy profile of the ligation bond was obtained as follows: first, we prepared for the QM/MM optimized geometry without constraints, and we used the resulting geometry as the initial geometry. Next, we moved the entire ligand atoms (i.e., side chain of His /Gln or water) along the [Mg atom of P_{D1}] – [N or O atom of the ligand head group] axis by 0.05 Å, optimized the geometry by constraining the distance between the Mg atom of P_{D1} and the N or O atom of the ligand head group, and calculated the energy of the resulting geometry. The axial ligands were also included in the QM region.

Computation of E_m(Chl*a*). The present computation was based on the electrostatic continuum model, wherein we solved the linear Poisson-Boltzmann equation with the MEAD program (*24*). To facilitate direct comparisons with previous computational results, identical computational conditions and parameters were used (e.g., Refs. (*7; 25; 26*)) such as atomic partial charges and dielectric constants. The redox states of all other cofactors (e.g., Pheo*a* and quinones) were kept in their neutral charge states during the redox titration of each Chl*a*. The ensemble of the protonation patterns was sampled using the Monte Carlo method with the Karlsberg program (*27*) (Rabenstein, B. *Karlsberg online manual*, http://agknapp.chemie.fu-berlin.de/karlsberg/ (1999)). The dielectric constants were set to $\varepsilon_p = 4$ inside the protein and $\varepsilon_w = 80$ for water. All computations were performed at 300 K, pH 7.0, and an ionic strength of 100 mM. The linear Poisson-Boltzmann equation was solved using a 3-step grid-focusing procedure at resolutions 2.5 Å, 1.0 Å, and 0.3 Å. The Monte Carlo sampling for a redox active group yielded the probabilities $[A_{ox}]$ and $[A_{red}]$ of the two redox states of the molecule A. E_m(Chl*a*) was evaluated using the Nernst equation. A bias potential was applied to obtain an equal amount of both redox states ($[A_{ox}] = [A_{red}]$), yielding the redox midpoint potential E_m as the resulting bias potential. For convenience, the computed E_m was given with mV accuracy without implying that the last digit is significant. In general, a few 10 mV in E_m is in a sufficiently reproducible range of our computational method.

E_m(Chl*a*) was measured to be +800 mV (versus normal hydrogen electrode) in CH_2Cl_2 with tetrabutylammonium perchlorate as the electrolyte (*28; 29*). Considering the solvation energy difference between CH_2Cl_2 and water, we used the value of +698 mV as a reference E_m(Chl*a*) value in water, as previously used in the wild type PSII (*7*). The axial ligands of the chlorophylls were not included in the reference model system mainly due to the absence of experimentally measured E_m values. Alternatively, they were considered as an external group that interacts with the chlorophyll electrostatically. Due to the following two reasons, only a Chl*a* molecule (without the axial ligand) was taken as a reference model system in the present study. (i) The same approaches were also employed by Gunner and coworkers, e.g., influence of the axial ligand on E_m(heme) of cytochromes (*8*). Because the reference model system does not contain a transition metal in the present study, the approximation of the ligand as an external group that influences electrostatically should be less crucial than that in the Fe-containing heme proteins. (ii) The calculated $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio and the spin density distribution are essentially the

same irrespective of the axial ligand being included in the MM region or the QM region (Table 1), suggesting that the influence of the axial ligand is predominantly due to its electrostatic effect rather than quantumchemical effect (see below).

RESULTS AND DISCUSSION

D1-H198Q mutant. In the O4H$^-$ O5H$^-$ OEC model, the $E_m(P_{D1})$ and $E_m(P_{D2})$ values for D1-H198Q mutant (Figure 1a) were calculated to be 1066 mV and 1168 mV, respectively (Table 1). Because the corresponding values were 1065 mV and 1166 mV for the wild type (*7*), it is clear that the values are not affected by the D1-H198Q mutation. This is in agreement with the experimental results showing that (i) the E_m values of P680/P680$^+$ remained unchanged upon D1-H198Q mutation in the *Synechocystis* PCC 6803 PSII (*5*); and (ii) the spectroscopic properties of P680$^{\bullet+}$ remained unaltered upon D1-H198Q mutation in the *T. elongatus* PSII (*10*). This, in turn, indicates that our calculation approach employed reflected the redox properties of P_{D1} and P_{D2} correctly. Because we did not observe any significant differences in the protonation states of titratable residues in the entire PSII, the influence of the axial ligands His and Gln on E_m should be essentially equal. Indeed, the direct influence of the Gln axial ligand on $E_m(P_{D1})$ was identical to that of the His axial ligand in the present PSII geometry, with a stabilization of the Chl*a* cationic state by ~70 mV (Table 2).

The lower value of $E_m(P_{D1})$ compared to $E_m(P_{D2})$ implies that a cationic state will be localized more in P_{D1} than P_{D2}. In agreement with the fact that the $E_m(P_{D1})$ and $E_m(P_{D2})$ values were identical between the D1-H198Q mutant and the wild type, the calculated $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio for the D1-H198Q mutant (77.0/23.0, Table 1) was unaltered as compared to that of the wild type PSII (76.9/23.1 (*7*)). The spin density distribution calculated for the wild type was 80.1/19.9, which is close to the experimentally obtained values (≈$P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio) of 82/18 from ENDOR studies of spinach PSII (*4*) or 80/20 from flash-induced spectroscopic studies of *Synechocystis* PCC 6803 PSII (*5*). In FTIR studies of *T. elongatus* PSII (*14; 15*), 70-80% of the cationic state was localized on one of the P_{D1}/P_{D2} Chl*a* units, which is also in agreement with the calculated $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio. In general, the spin density distribution is significantly affected by the spin polarization of the energetically low spin-paired π-orbitals, which tends to reduce small spin densities (*30*). Thus, the calculated spin density distribution was more asymmetric than that of the charge distribution (Table 1), a fact already pointed out previously (*15; 30*).

The calculated $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio and the spin density distribution are essentially the same irrespective of the axial ligand being included in the MM region or the QM region (Table 1), suggesting that the influence of axial ligand is predominantly due to its electrostatic effect rather than quantumchemical effect.

D1-H198A mutant. A simple replacement of D1-His198 with Ala (**D1-H198A without a water ligand**) resulted in a 47-mV increase in the $E_m(P_{D1})$ value (Table 1). The $E_m(P_{D2})$ value also increased by 16 mV by replacing D1-H198 with Ala (Table 1). His ligands are widely known to decrease E_m of hemes in heme proteins and model systems (*8*). The larger shift observed in $E_m(P_{D1})$ resulted in a more equipotential in the $E_m(P_{D1})/E_m(P_{D2})$ pair in the D1-H198A mutant ($E_m(P_{D2}) - E_m(P_{D1})$ = 70 mV) than that in the wild type PSII (100 mV). Therefore, the positive charge will shift to a greater extent onto P_{D2}, yielding a calculated $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio of 68.5/31.5 for the D1-H198A mutant in the absence of a water ligand (Table 1). The spectroscopic properties of P680$^{\bullet+}$, however, have been reported to be unchanged upon the D1-H198A mutation in *T. elongatus* PSII (*10*). Thus, it appears that the present structural model, D1-H198A mutant without a water ligand, does not adequately describe the features of the actual D1-H198A mutant.

Analogous to the His axial ligand replacement with Gly in PbRC (*31*) and PSI (*32*), Diner et al. proposed that the D1-His198A mutant might possess a water molecule as an axial ligand for P_{D1} (*5*).

Thus far, this water molecule has not been detected in FTIR studies (*10*) because of the difficulty in exchanging water molecules possibly serving as the axial ligands for P_{D1}. However, P_{D1} has been confirmed to be a chlorophyll, not a pheophytin, in the D1-H198A mutant based on the unchanged P680/P680$^+$ FTIR spectra (*10*). A water molecule as an axial ligand can be seen in the accessory chlorophylls in PSII: (a) Chl_{D1} (the axial water H-bonded with another molecule of water that is further H-bonded to both the backbone carbonyl (C=O) of D1-Ile176 and also to the side chain OH of D1-Thr179 and (b) Chl_{D2} (the axial water H-bonded with another water molecule that is in turn H-bonded to the backbone C=O of D2-Val175 (*13*). Similar interactions can be observed in the accessory chlorophylls in PSI, A_{-1A} (with the side chain C=O of PsaA-Asn604) and A_{-1B} (with the side chain C=O of PsaB-Asn591) (*33*). We therefore introduced two water molecules in the D1-H198A mutant: one acts as the axial ligand to P_{D1} (Mg^{2+}–O_{water} distance = 2.0 Å), and the other one is H-bonded with the first one (O_{water}–O_{water} distance = 2.5 Å) (Figure 1b). The position of the second water molecule was fixed by forming H-bonds with both the backbone C=O of D1-Ala198 ($O_{D1\text{-}A198}$–O_{water} distance = 3.1 Å), and a crystal water (O_{water}–O_{water} distance = 2.6 Å) which is found in the 1.9 Å structure and forms an H-bond with the keto C=O of Chl_{D2} (O_{water}–O_{ChlD2} distance = 2.8 Å) (*13*). Thus a well-ordered H-bond network between P_{D1} and Chl_{D2} can be seen in the **D1-H198A mutant with a water ligand** (Figure 1b). The potential-energy profile of the water ligand with respect to the Mg–O_{water} distance is close to that of the Gln ligand rather than the His ligand (Figure 2), probably because the head group atom is O in both water and Gln in contrast to N in His.

Using this geometry, we calculated $E_m(P_{D1})$ and $E_m(P_{D2})$ for the D1-H198A mutant with a water ligand to be 1054 mV and 1164 mV, respectively (Table 1). This yields $E_m(P_{D2}) - E_m(P_{D1})$ = 110 mV, which is closer to the corresponding value for the wild type (100 mV) than the value for the D1-H198A mutant without a water ligand (70 mV). Furthermore, the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio was calculated to be 77.0/23.0, which is similar to the value of 76.9/23.1 for the wild type, but considerably different from the value (68.5/31.5) calculated for the D1-H198A mutant without a water ligand (Table 1). If the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio were altered to 68.5/31.5 upon the D1-H198A mutation, the FTIR spectra for the *T. elongatus* PSII (*10*) would be expected to be significantly different from those of the wild type, which is not the case. Hence, the unchanged redox and spectroscopic properties of P680 in *T. elongatus* PSII (*10*) can be best explained by the presence of a water molecule as the axial ligand for P_{D1} in the D1-H198A mutant, in agreement with that proposed by Diner et al. (*5*).

D1-H198A mutant of *Synechocystis* PCC 6803 PSII. The presence of a water molecule as the axial ligand of P_{D1} in the D1-H198A mutant was originally proposed in studies of the *Synechocystis* PCC 6803 PSII (*5*). However, in contrast to *T. elongatus*, $E_m(P_{D1})$ in the D1-H198A mutant were –74 and –84 mV lower than that in the native PSII in whole cells (where the OEC cluster is present) and the "Mn-depleted PSII" core complexes of *Synechocystis* PCC 6803, respectively (*5*). To explain the significantly lowered $E_m(P_{D1})$ in the D1-H198A mutant, the ligand water molecule of P_{D1} was proposed to be OH^- in the P680$^{\bullet+}$ state of the *Synechocystis* PCC 6803 PSII (*5*). In the protein environment of PSII from *T. vulcanus* (*13*), however, $E_m(P_{D1})$ calculated in the presence of the fully ionized OH^- axial ligand in the D1-H198A mutant was unusually low, 450 mV lower than the native PSII due to the proximity of the negative charge to $P_{D1}^{\bullet+}$ (Table 1). The unusually lowered $E_m(P_{D1})$ of 604 mV suggests that the ligand water molecule cannot be deprotonated in response to the $P_{D1}^{\bullet+}$ formation on the basis of the *T. vulcanus* PSII crystal structure. Hence, the fully ionized OH^- axial ligand is unlikely to be relevant for the D1-H198A mutant PSII of *T. vulcanus* on the basis of the crystal structure. Possibly in the *Synechocystis* PCC 6803 PSII, ~20 % deprotonation of the H_2O ligand (i.e., $OH^{-0.2}$) might account for the $E_m(P_{D1})$ downshift of ~80 mV upon D1-H198A mutation (*5*). In general, deprotonation of H_2O is energetically possible only in the proximity of highly positively charged groups because $pK_a(H_2O/OH^-)$ is significantly high, ~16 in aqueous solution. The coordination of H_2O on Mg^{2+} of the positively

charged $P_{D1}^{\bullet+}$ will contribute to the decrease in $pK_a(H_2O/OH^-)$, which may result in partial deprotonation of the H_2O ligand possibly through the displacement of an H bond to the protein (*5*).

In the neighborhood of P_{D1}/P_{D2}, there exist the lumenal α-helices **cd** of D1, which play a crucial role in the energetics of $[P_{D1}/P_{D2}]^{\bullet+}$ (*7; 25; 34-36*). The protein primary sequences of the lumenal α-helices **cd** of D1 are identical among *T. elongatus* and *Synechocystis* PCC 6803. On the other hand, a notable difference is observed at D1-199, next to the P_{D1} axial ligand (D1-His198) in the transmembrane α-helices **d**, where Gln is situated in *T. elongatus* but is replaced with Met in *Synechocystis* PCC 6803. This might result in the different binding modes of the axial water ligand at P_{D1} between *T. elongatus* and *Synechocystis* PCC 6803. However, the absence of the latter PSII crystal structure hinders us to speculate further details, as previously concluded in the studies of the *T. elongatus* PSII (*10*).

In summary, the presence of a H_2O axial ligand rather than an ionized OH^- ligand, appears to be the case with the D1-H198A mutant in the geometry of the *T. vulcanus* crystal structure (*13*), in terms of $E_m(P_{D1})$ measured in the *T. elongatus* PSII (*10*) and the apparently large structural similarity between the *T. elongatus* (*11; 12*) and *T. vulcanus* PSII (*13*).

CONCLUSIONS

The D1-H198Q mutation altered neither E_m for P_{D1} and P_{D2} nor the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio: thus explaining the unaffected spectroscopic properties of P680 in PSII from *T. elongatus* (*10*) and the unchanged values of E_m for $P680/P680^+$ in PSII from *Synechocystis* PCC 6803 (*5*). Replacing His with Ala at the D1-198 position resulted in a significant increase of ~50 mV in $E_m(P_{D1})$, leading to a decrease in the $P_{D1}^{\bullet+}$ state to 68% compared with 77 % in the wild type, if no water ligands are introduced. When a water molecule was introduced to serve as the axial ligand for P_{D1} in the D1-H198A mutant (originally proposed by Diner et al. (*5*) while not detected in experimental studies so far (*10*)), the replacement of His by Ala resulted in little effect on either E_m or the $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio, in agreement with the experimental results reported. The present study demonstrated the existence of a H-bond network in the mutant which proceeds from the ligand water of P_{D1} to the chlorin ring of Chl_{D2} in which, the water ligand was geometrically maintained by a second water molecule that formed H bonds with (i) the backbone C=O of D1-Ala198 and (ii) a crystal water that is in turn H-bonded to the keto C=O of Chl_{D2}.

ACKNOWLEDGMENT

This research was supported by the JST PRESTO program (H.I), Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan (22740276 to K.S.), Special Coordination Fund (H.I) for Promoting Science and Technology of MEXT, Takeda Science Foundation (H.I.), Kyoto University Step-up Grant-in-Aid for young scientists (H. I.), and Grant for Basic Science Research Projects from The Sumitomo Foundation (H. I.).

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TABLE 1. Calculated values of $E_m(P_{D1})$, $E_m(P_{D2})$ (in mV), $P_{D1}^{\bullet+}/P_{D2}^{\bullet+}$ ratio, and spin density distribution in the O4H$^-$ O5H$^-$ OEC model (in %). The axial ligand was included either in the MM region or in QM region. The latter considers the axial ligand quantumchemically. $\Delta E_m = E_m(P_{D2}) - E_m(P_{D1})$; +/–$H_2O$ = presence/absence of H_2O as the P_{D1} axial ligand; +OH^- = presence of fully ionized OH^- as the P_{D1} axial ligand.

Axial ligand				**in MM region**				**in QM region**			
	E_m			**charge**		**spin**		**charge**		**spin**	
	P_{D1}	P_{D2}	ΔE_m	$P_{D1}^{\bullet+}$	$P_{D2}^{\bullet+}$	P_{D1}	P_{D2}	$P_{D1}^{\bullet+}$	$P_{D2}^{\bullet+}$	P_{D1}	P_{D2}
wild type [a]	1065	1166	101	76.9	23.1	80.6	19.4	73.9	26.1	81.1	18.9
D1-H198Q	1066	1168	102	77.0	23.0	75.6	24.4	75.9	24.1	78.9	21.1
D1-H198A											
+ H_2O	1054	1164	110	77.0	23.0	81.2	18.8	77.3	22.7	80.5	19.5
– H_2O	1112	1182	70	68.5	31.5	68.4	31.6	62.9	37.1	60.8	39.2
+ OH^- [c]	604	967	363	103.2	-3.2	98.5	1.5	n.d. [b]	n.d. [b]	n.d. [b]	n.d. [b]

[a] See Ref. (*7*).

[b] Not determined due to the unusually large displacement of the Mg atom from the P_{D1} chlorin plane in the QM/MM geometry optimized structure.

[c] Fully ionized state.

TABLE 2. Direct influence of the axial ligand on the $E_m(P_{D1})$ shift (in mV) by considering the chromophore and its direct ligand only.

	Axial ligand	**$\Delta E_m(P_{D1})$**
wild type	His	-73
D1-H198Q	Gln	-73
D1-H198A		
+ H_2O	Ala + axial H_2O	-53
	Ala + axial & H-bonded H_2O	-83
– H_2O	Ala	3

FIGURE CAPTIONS

FIGURE 1: (a) QM/MM optimized geometry of the D1-H198Q mutant. (b) Arrangement of water molecules and the H-bond network in the D1-H198A mutant (with a water ligand). Oxygen (red) atoms of water molecules, oxygen and nitrogen (blue) atoms of D1-198, and Mg (pink) atoms of P_{D1}, P_{D2} and Chl_{D2} chlorophylls are depicted as balls.

FIGURE 2: Potential-energy profiles of the ligation bond along the [Mg atom of P_{D1}] – [N or O atom of the axial ligand] axis in the wild type (black, energy minimum at 2.10 Å), D1-H198Q (blue, energy minimum at 1.98 Å), D1-H198A with a water ligand (red, energy minimum at 2.02 Å) PSII proteins. The axial ligands were included in the QM region.

Figure 1.

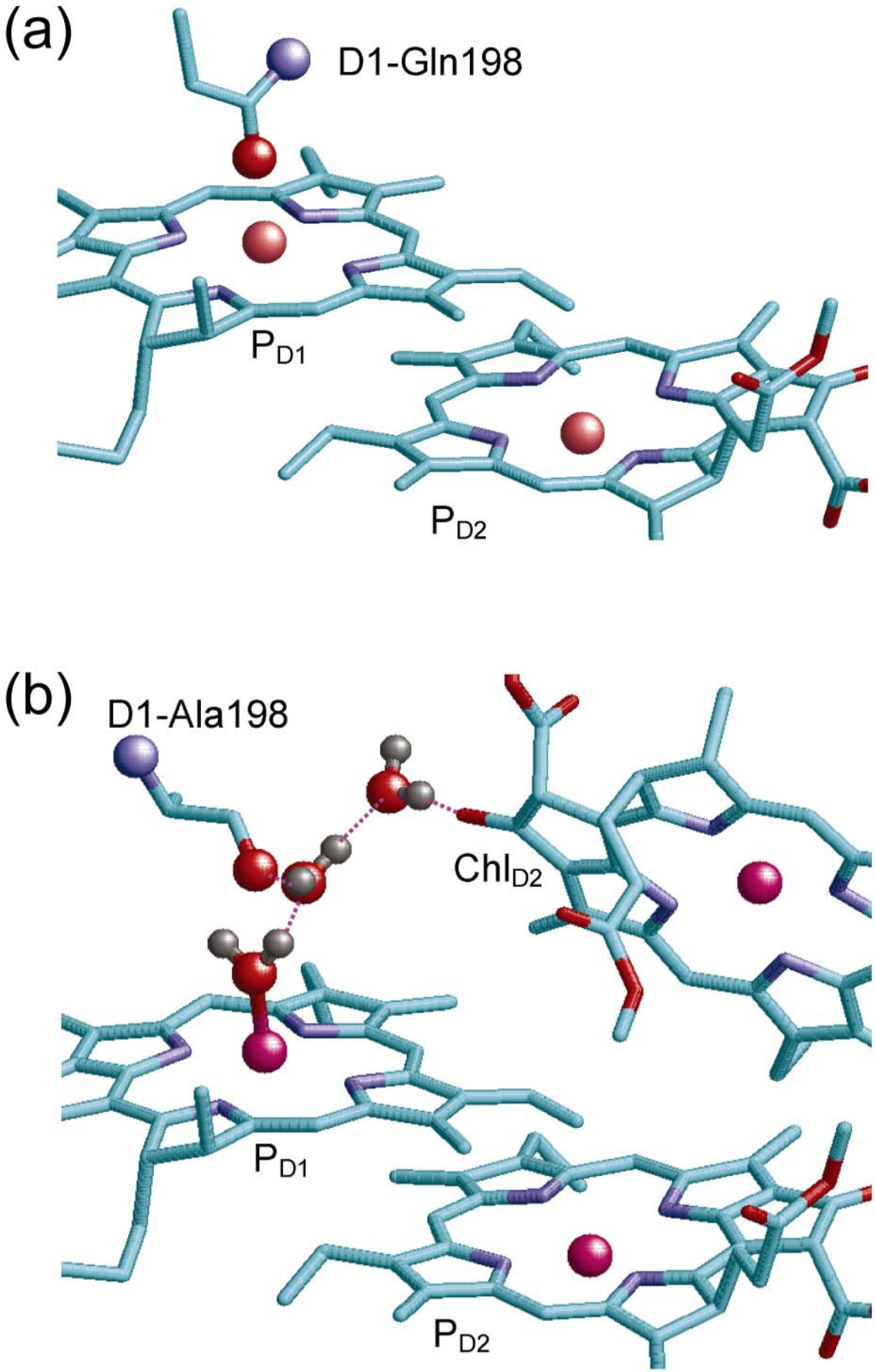
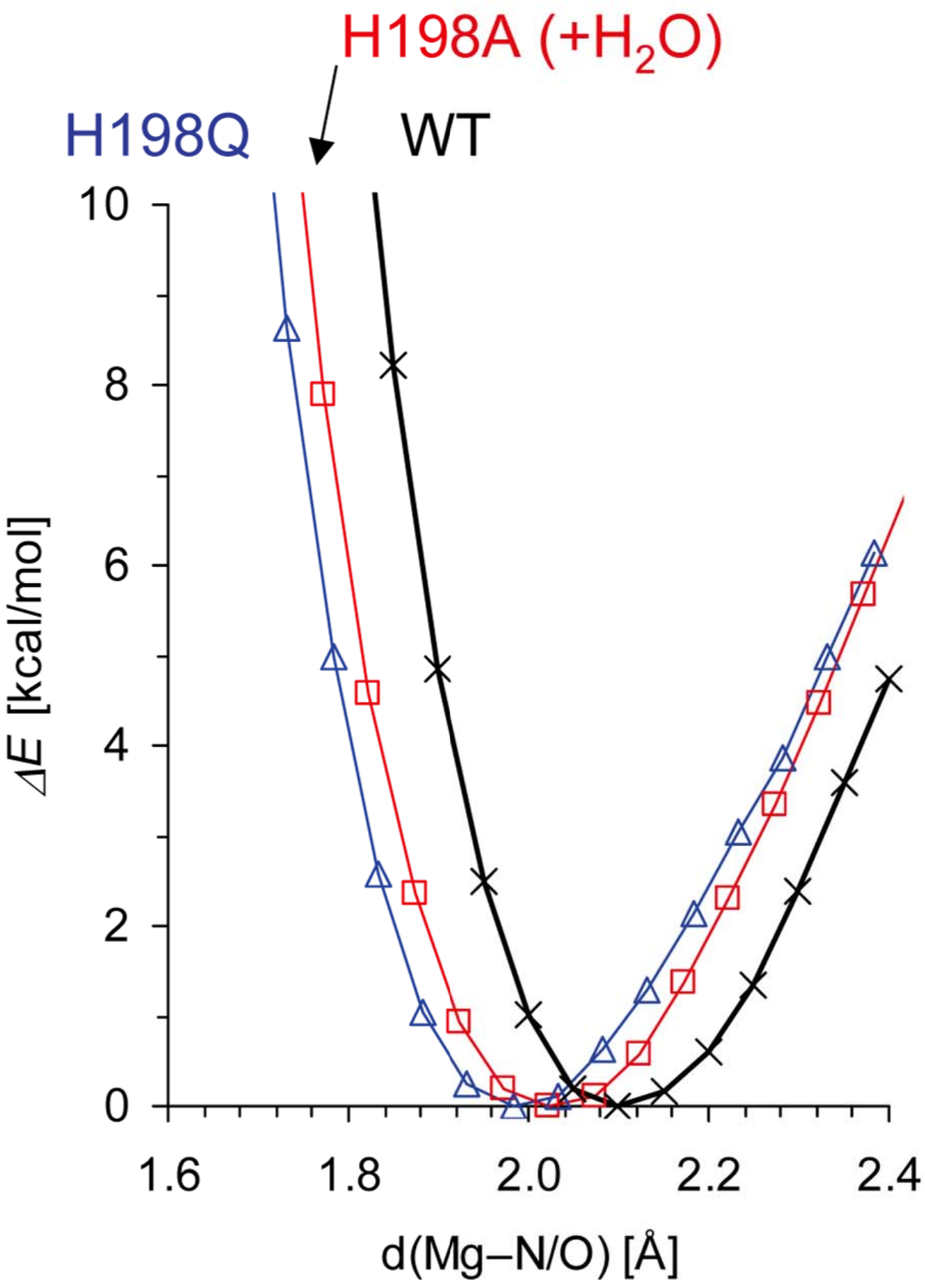


Figure 2.



Influence of the axial ligand on the cationic properties of the chlorophyll pair in photosystem II from *Thermosynechococcus vulcanus*

Keisuke Saito, Jian-Ren Shen, and Hiroshi Ishikita

Table S1. Atomic charges (**ESP: unrestricted DFT**) and coordinates of the QM/MM optimized geometry.

(a) Atomic charges in calculations with axial ligands in MM region.

	atom	Wild type	D1-H198Q	D1-H198A with H_2O	D1-H198A without H_2O	D1-H198A with OH^-
PD1	MG	1.55276	1.50969	1.49284	1.02109	1.9625
PD1	CHA	-0.18538	-0.14226	-0.14698	-0.01855	-0.21332
PD1	CHB	-0.49704	-0.47702	-0.48684	-0.36425	-0.58233
PD1	HHB	0.16279	0.16033	0.1619	0.14776	0.15785
PD1	CHC	-0.48553	-0.45021	-0.44678	-0.30134	-0.6013
PD1	HHC	0.1941	0.19917	0.18605	0.16438	0.21154
PD1	CHD	-0.57747	-0.56898	-0.59905	-0.40039	-0.73806
PD1	HHD	0.25481	0.25075	0.26545	0.22676	0.26929
PD1	NA	-0.59333	-0.55279	-0.54799	-0.30801	-0.73446
PD1	C1A	0.19607	0.15615	0.17659	-0.02736	0.3384
PD1	C2A	0.0071	-0.03121	-0.01066	0.00647	-0.04955
PD1	H2A	0.06523	0.07988	0.07264	0.06966	0.06806
PD1	C3A	0.07605	0.13277	0.09788	0.17451	0.11197
PD1	H3A	0.02532	0.01823	0.02449	0.0162	0.00636
PD1	C4A	0.43304	0.37606	0.39798	0.19913	0.50781
PD1	CMA	-0.39752	-0.41566	-0.40507	-0.42378	-0.4186
PD1	HMA1	0.09769	0.10101	0.09917	0.10093	0.08987
PD1	HMA2	0.12466	0.12859	0.12563	0.14083	0.14587
PD1	HMA3	0.10739	0.10961	0.10699	0.11121	0.11025
PD1	CAA	0.21871	0.14791	0.2113	0.13291	0.1596
PD1	HAA1	-0.01097	0.01408	-0.00944	0.01485	0.01706
PD1	HAA2	0.02096	0.04092	0.02315	0.04396	0.02931
PD1	CBA	-0.60216	-0.56108	-0.59325	-0.54872	-0.55432
PD1	HBA1	0.13102	0.12275	0.12833	0.11958	0.11913
PD1	HBA2	0.173	0.16848	0.17216	0.16456	0.15846
PD1	CGA	0.7933	0.79051	0.79126	0.78486	0.80014
PD1	O1A	-0.49258	-0.49416	-0.49244	-0.48741	-0.49863
PD1	O2A	-0.37316	-0.37759	-0.37314	-0.37762	-0.38594
PD1	NB	-0.81517	-0.74914	-0.76229	-0.49447	-1.05383

PD1	C1B	0.35821	0.33118	0.33651	0.19365	0.5479
PD1	C2B	0.17823	0.17579	0.17765	0.18531	0.16424
PD1	C3B	-0.24919	-0.22365	-0.21527	-0.15897	-0.29078
PD1	C4B	0.55073	0.50012	0.52078	0.31227	0.72965
PD1	CMB	-0.42315	-0.41613	-0.42422	-0.40316	-0.43241
PD1	HMB1	0.10854	0.10649	0.10808	0.10787	0.10838
PD1	HMB2	0.14803	0.14922	0.14786	0.14592	0.15379
PD1	HMB3	0.13567	0.12964	0.13706	0.12118	0.12233
PD1	CAB	0.02407	0.01085	0.00279	-0.00184	0.0598
PD1	HAB	0.07777	0.08252	0.08501	0.08824	0.07256
PD1	CBB	-0.37325	-0.36917	-0.36361	-0.37542	-0.41049
PD1	HBB1	0.15493	0.15487	0.15352	0.15784	0.1621
PD1	HBB2	0.14553	0.14351	0.14184	0.1433	0.15416
PD1	NC	-0.81539	-0.81671	-0.80223	-0.55691	-1.02582
PD1	C1C	0.42229	0.4013	0.40371	0.24601	0.62844
PD1	C2C	0.06265	0.12627	0.06726	0.10143	0.10354
PD1	C3C	-0.25988	-0.27776	-0.27129	-0.1593	-0.32113
PD1	C4C	0.62936	0.62286	0.62399	0.39601	0.81774
PD1	CMC	-0.19773	-0.4326	-0.2026	-0.23869	-0.41614
PD1	HMC1	0.01665	0.13085	0.01473	0.02784	0.11417
PD1	HMC2	0.08162	0.09069	0.08785	0.09822	0.08839
PD1	HMC3	0.11854	0.1844	0.11781	0.12074	0.17845
PD1	CAC	0.03178	0.06862	0.05784	-0.00434	0.04929
PD1	HAC1	0.08023	0.06696	0.07251	0.08533	0.08038
PD1	HAC2	0.04143	0.03159	0.03162	0.05299	0.03628
PD1	CBC	-0.13674	-0.14513	-0.12496	-0.14858	-0.17179
PD1	HBC1	0.01115	0.0199	0.00442	0.01725	0.02937
PD1	HBC2	0.08948	0.08977	0.08483	0.09656	0.08888
PD1	HBC3	0.04759	0.04726	0.04585	0.04905	0.05136
PD1	ND	-0.91552	-0.91349	-0.87948	-0.55945	-1.19368
PD1	C1D	0.57642	0.56564	0.54941	0.32703	0.84082
PD1	C2D	0.04892	0.05527	0.06347	0.10882	-0.03486
PD1	C3D	-0.29075	-0.29873	-0.30803	-0.23298	-0.3104
PD1	C4D	0.50592	0.51828	0.48299	0.26683	0.7037
PD1	CMD	-0.4552	-0.45272	-0.45321	-0.44502	-0.41782
PD1	HMD1	0.13311	0.13242	0.12978	0.13603	0.11666

PD1	HMD2	0.19471	0.1954	0.19007	0.19594	0.19398
PD1	HMD3	0.17506	0.17271	0.17886	0.16163	0.15466
PD1	CAD	0.69542	0.69454	0.7164	0.63101	0.71713
PD1	OBD	-0.45896	-0.45694	-0.46413	-0.44515	-0.469
PD1	CBD	-0.67532	-0.70748	-0.68648	-0.60353	-0.79492
PD1	HBD1	0.19965	0.2062	0.19948	0.17284	0.21552
PD1	CGD	0.88215	0.89706	0.86928	0.89816	0.93292
PD1	O1D	-0.59143	-0.59005	-0.58256	-0.58728	-0.58075
PD1	O2D	-0.32648	-0.32373	-0.32201	-0.33636	-0.32745
PD1	CED	-0.15401	-0.16809	-0.15578	-0.17025	-0.18078
PD1	HED1	0.10968	0.11158	0.11051	0.1138	0.11671
PD1	HED2	0.12007	0.12204	0.11961	0.12196	0.11835
PD1	HED3	0.12398	0.12811	0.12397	0.13037	0.12198
PD1	C1	-0.10682	-0.09819	-0.10785	-0.10015	-0.08906
PD1	H1	0.12411	0.12227	0.12461	0.12338	0.12384
PD1	H2	0.09855	0.09639	0.09886	0.09815	0.08691
PD1	H3	0.09321	0.09081	0.09334	0.09193	0.08164
PD2	MG	1.31365	1.34062	1.31991	1.32684	1.32046
PD2	CHA	0.0966	0.07654	0.09152	0.08946	0.08104
PD2	CHB	-0.43224	-0.44094	-0.43697	-0.42699	-0.44084
PD2	HHB	0.14966	0.14994	0.14945	0.14953	0.14252
PD2	CHC	-0.18604	-0.24443	-0.19855	-0.23882	-0.27865
PD2	HHC	0.14632	0.1575	0.14221	0.15033	0.18617
PD2	CHD	-0.51906	-0.50757	-0.52163	-0.53006	-0.48679
PD2	HHD	0.22033	0.21603	0.22051	0.21994	0.21485
PD2	NA	-0.28956	-0.3218	-0.29886	-0.30055	-0.32296
PD2	C1A	-0.19439	-0.16604	-0.18677	-0.17675	-0.18825
PD2	C2A	0.16774	0.17156	0.15801	0.17837	0.15693
PD2	H2A	-0.00538	-0.00543	-0.0031	-0.00473	-0.0086
PD2	C3A	0.34877	0.33612	0.35162	0.33395	0.34688
PD2	H3A	-0.05491	-0.05212	-0.05604	-0.04845	-0.0572
PD2	C4A	0.06987	0.09686	0.07752	0.08321	0.09296
PD2	CMA	-0.42871	-0.4289	-0.42899	-0.42826	-0.43454
PD2	HMA1	0.07821	0.07952	0.07766	0.08105	0.07235
PD2	HMA2	0.10058	0.0995	0.10064	0.09981	0.10007

PD2	HMA3	0.12419	0.12511	0.12413	0.12569	0.12209
PD2	CAA	0.17249	0.16399	0.17759	0.14861	0.20718
PD2	HAA1	0.01619	0.0186	0.01567	0.02327	0.01313
PD2	HAA2	-0.00093	0.0016	-0.00213	0.00613	-0.0144
PD2	CBA	-0.67927	-0.67793	-0.68016	-0.67228	-0.68995
PD2	HBA1	0.15957	0.15981	0.15962	0.15969	0.15524
PD2	HBA2	0.1557	0.15618	0.15594	0.15517	0.15452
PD2	CGA	0.84711	0.8463	0.84663	0.84488	0.84685
PD2	O1A	-0.55005	-0.54934	-0.55008	-0.54779	-0.5523
PD2	O2A	-0.34255	-0.34253	-0.34243	-0.34244	-0.34158
PD2	NB	-0.48556	-0.51067	-0.49556	-0.50938	-0.49396
PD2	C1B	0.24953	0.25393	0.25184	0.25576	0.23047
PD2	C2B	0.0474	0.07208	0.05095	0.0598	0.08966
PD2	C3B	0.02807	-0.04175	0.0116	0.00299	-0.07283
PD2	C4B	0.07005	0.13473	0.09287	0.12438	0.1452
PD2	CMB	-0.29184	-0.28772	-0.29292	-0.30384	-0.27657
PD2	HMB1	0.0682	0.06835	0.06779	0.07449	0.06575
PD2	HMB2	0.09098	0.08824	0.0911	0.09456	0.07727
PD2	HMB3	0.08264	0.08111	0.0832	0.08753	0.07488
PD2	CAB	-0.08565	-0.00788	-0.07353	-0.0829	0.00389
PD2	HAB	0.06514	0.00574	0.06574	0.05328	0.01029
PD2	CBB	-0.33939	-0.35016	-0.34583	-0.31971	-0.36182
PD2	HBB1	0.13859	0.13734	0.14062	0.1319	0.13376
PD2	HBB2	0.15854	0.15987	0.15944	0.15769	0.15484
PD2	NC	-0.5127	-0.54715	-0.51725	-0.5464	-0.53962
PD2	C1C	0.10544	0.16392	0.09859	0.17841	0.16797
PD2	C2C	0.14228	0.13298	0.16354	0.07696	0.09887
PD2	C3C	-0.23176	-0.29539	-0.23054	-0.20502	-0.28069
PD2	C4C	0.42023	0.43165	0.42245	0.43851	0.39787
PD2	CMC	-0.39279	-0.3593	-0.43886	-0.323	-0.31008
PD2	HMC1	0.09282	0.07415	0.1165	0.05062	0.05591
PD2	HMC2	0.10027	0.09504	0.11257	0.09324	0.07637
PD2	HMC3	0.16247	0.15863	0.16774	0.15284	0.14476
PD2	CAC	0.23256	0.29796	0.2282	0.22534	0.30333
PD2	HAC1	0.01462	0.00774	0.01593	0.01841	0.00164
PD2	HAC2	0.01924	0.00484	0.02134	0.02266	0.00126

PD2	CBC	-0.38701	-0.42313	-0.38708	-0.3941	-0.42174
PD2	HBC1	0.08497	0.09107	0.08512	0.08802	0.08704
PD2	HBC2	0.13142	0.13662	0.13148	0.13603	0.12742
PD2	HBC3	0.0874	0.10182	0.08713	0.08838	0.09849
PD2	ND	-0.6268	-0.6494	-0.63248	-0.64292	-0.62145
PD2	C1D	0.36846	0.3774	0.37333	0.39653	0.33525
PD2	C2D	0.10574	0.10455	0.10249	0.10214	0.09842
PD2	C3D	-0.30573	-0.30932	-0.30336	-0.30454	-0.30988
PD2	C4D	0.18826	0.21365	0.19184	0.20109	0.18802
PD2	CMD	-0.38338	-0.3845	-0.38248	-0.38409	-0.37451
PD2	HMD1	0.14182	0.14367	0.14231	0.1458	0.13748
PD2	HMD2	0.11474	0.11535	0.11434	0.11719	0.10564
PD2	HMD3	0.15875	0.15976	0.15862	0.16106	0.14951
PD2	CAD	0.72407	0.7257	0.72109	0.7275	0.72035
PD2	OBD	-0.48123	-0.47954	-0.48112	-0.47559	-0.49946
PD2	CBD	-0.69427	-0.69091	-0.68974	-0.69104	-0.69125
PD2	HBD1	0.20018	0.19969	0.19955	0.19963	0.19892
PD2	CGD	0.83747	0.83435	0.83526	0.83262	0.83144
PD2	O1D	-0.55426	-0.55375	-0.55386	-0.55271	-0.55596
PD2	O2D	-0.36564	-0.36425	-0.36533	-0.36192	-0.36811
PD2	CED	-0.1001	-0.10128	-0.10029	-0.1053	-0.08551
PD2	HED1	0.12108	0.1219	0.12126	0.12329	0.1153
PD2	HED2	0.10502	0.10614	0.10536	0.10833	0.0978
PD2	HED3	0.11653	0.11701	0.11592	0.11879	0.10471
PD2	C1	-0.10219	-0.10248	-0.1027	-0.10405	-0.09821
PD2	H1	0.08301	0.08355	0.08304	0.08468	0.07682
PD2	H2	0.11522	0.11543	0.11549	0.11692	0.1167
PD2	H3	0.11391	0.11427	0.11409	0.11503	0.10921

total (PD1)	0.76931	0.7696	0.77033	0.68526	1.03187
total (PD2)	0.23071	0.2304	0.22972	0.3147	-0.03196

(b) Atomic charges in calculations with axial ligands in MM region.

	residue	atom	Wild type	D1-H198Q	D1-H198A with H_2O	D1-H198A without H_2O
PD1	CLA	4MG	0.5633	0.7813	1.1205	1.0205
PD1	CLA	4 CHA	0.0126	-0.1159	-0.1092	-0.0154
PD1	CLA	4 CHB	-0.2573	-0.3454	-0.3804	-0.3652
PD1	CLA	4 HHB	0.1387	0.1463	0.1403	0.1467
PD1	CLA	4 CHC	-0.2707	-0.2307	-0.296	-0.3023
PD1	CLA	4 HHC	0.1461	0.1333	0.1385	0.1538
PD1	CLA	4 CHD	-0.3601	-0.4162	-0.5361	-0.4034
PD1	CLA	4 HHD	0.2202	0.2303	0.2478	0.2269
PD1	CLA	4 NA	-0.2282	-0.3237	-0.4015	-0.3072
PD1	CLA	4 C1A	-0.0065	0.0524	0.0565	-0.0274
PD1	CLA	4 C2A	0.0085	0.0277	0.058	-0.0119
PD1	CLA	4 H2A	0.0766	0.0626	0.0605	0.075
PD1	CLA	4 C3A	0.1231	0.0916	0.0515	0.1842
PD1	CLA	4 H3A	0.0321	0.0357	0.032	0.0132
PD1	CLA	4 C4A	0.1181	0.2221	0.3229	0.1912
PD1	CLA	4 CMA	-0.3817	-0.4313	-0.3761	-0.4259
PD1	CLA	4HMA1	0.0924	0.1013	0.0883	0.1
PD1	CLA	4HMA2	0.117	0.1462	0.1242	0.1411
PD1	CLA	4HMA3	0.1045	0.117	0.103	0.1114
PD1	CLA	4 CAA	0.1456	0.2444	0.2354	0.1358
PD1	CLA	4HAA1	0.032	-0.0065	-0.0206	0.0155
PD1	CLA	4HAA2	0.0406	0.0217	0.0185	0.0429
PD1	CLA	4 CBA	-0.5822	-0.6413	-0.6088	-0.5463
PD1	CLA	4HBA1	0.1237	0.135	0.13	0.1189
PD1	CLA	4HBA2	0.1715	0.1818	0.1747	0.1636
PD1	CLA	4 CGA	0.7973	0.8018	0.7886	0.7837
PD1	CLA	4 O1A	-0.4952	-0.4982	-0.4928	-0.4873
PD1	CLA	4 O2A	-0.3745	-0.3681	-0.3717	-0.3778
PD1	CLA	4 NB	-0.4015	-0.4248	-0.4883	-0.4966
PD1	CLA	4 C1B	0.0519	0.1991	0.2027	0.1904
PD1	CLA	4 C2B	0.2604	0.1597	0.1709	0.1936
PD1	CLA	4 C3B	-0.2195	-0.1332	-0.1395	-0.1616
PD1	CLA	4 C4B	0.3416	0.2632	0.3025	0.3117

PD1	CLA	4	CMB	-0.4285	-0.4038	-0.4008	-0.4122
PD1	CLA	4	HMB1	0.1048	0.1009	0.1016	0.1072
PD1	CLA	4	HMB2	0.1418	0.143	0.1404	0.1465
PD1	CLA	4	HMB3	0.1432	0.1346	0.1357	0.1304
PD1	CLA	4	CAB	-0.0239	-0.0596	-0.0435	-0.0333
PD1	CLA	4	HAB	0.1002	0.1113	0.1073	0.105
PD1	CLA	4	CBB	-0.3131	-0.298	-0.311	-0.3068
PD1	CLA	4	HBB1	0.1296	0.1271	0.1288	0.1269
PD1	CLA	4	HBB2	0.1296	0.1256	0.1283	0.1234
PD1	CLA	4	NC	-0.363	-0.44	-0.6583	-0.5508
PD1	CLA	4	C1C	0.1446	0.1476	0.3013	0.2445
PD1	CLA	4	C2C	0.0915	0.1889	0.0674	0.089
PD1	CLA	4	C3C	-0.2019	-0.2466	-0.2317	-0.1591
PD1	CLA	4	C4C	0.3469	0.3975	0.5286	0.3854
PD1	CLA	4	CMC	-0.1826	-0.4501	-0.1855	-0.2198
PD1	CLA	4	HMC1	0.0084	0.1227	0.01	0.0203
PD1	CLA	4	HMC2	0.0794	0.1055	0.0877	0.1047
PD1	CLA	4	HMC3	0.1069	0.1805	0.1035	0.1052
PD1	CLA	4	CAC	0.0648	0.0979	0.049	0.0143
PD1	CLA	4	HAC1	0.0607	0.0522	0.0696	0.0807
PD1	CLA	4	HAC2	0.0332	0.0237	0.0342	0.0461
PD1	CLA	4	CBC	-0.141	-0.1472	-0.1271	-0.154
PD1	CLA	4	HBC1	0.0143	0.0189	0.0105	0.0237
PD1	CLA	4	HBC2	0.0865	0.0859	0.0833	0.0951
PD1	CLA	4	HBC3	0.0461	0.0451	0.0449	0.048
PD1	CLA	4	ND	-0.4331	-0.4964	-0.7594	-0.559
PD1	CLA	4	C1D	0.2529	0.3148	0.4971	0.3278
PD1	CLA	4	C2D	0.1602	0.1119	0.0661	0.1023
PD1	CLA	4	C3D	-0.3215	-0.2743	-0.2994	-0.231
PD1	CLA	4	C4D	0.2851	0.3082	0.4507	0.2584
PD1	CLA	4	CMD	-0.4582	-0.4441	-0.4519	-0.4416
PD1	CLA	4	HMD1	0.1348	0.1319	0.1294	0.1349
PD1	CLA	4	HMD2	0.1865	0.1835	0.1896	0.194
PD1	CLA	4	HMD3	0.1694	0.1672	0.174	0.1594
PD1	CLA	4	CAD	0.7033	0.6657	0.6929	0.6309
PD1	CLA	4	OBD	-0.4654	-0.4631	-0.4622	-0.448

PD1	CLA	4	CBD	-0.6723	-0.5705	-0.6724	-0.6038
PD1	CLA	4	HBD1	0.1888	0.1703	0.194	0.173
PD1	CLA	4	CGD	0.8641	0.8476	0.882	0.8948
PD1	CLA	4	O1D	-0.5836	-0.5863	-0.5875	-0.5857
PD1	CLA	4	O2D	-0.3166	-0.3226	-0.3273	-0.3367
PD1	CLA	4	CED	-0.1645	-0.1536	-0.1584	-0.1665
PD1	CLA	4	HED1	0.1098	0.1085	0.1098	0.1125
PD1	CLA	4	HED2	0.1211	0.1184	0.1188	0.1198
PD1	CLA	4	HED3	0.1264	0.123	0.1248	0.1291
PD1	CLA	4	C1	-0.1065	-0.1137	-0.1058	-0.0999
PD1	CLA	4	H1	0.1237	0.1258	0.1237	0.1232
PD1	CLA	4	H2	0.0978	0.0981	0.0971	0.0973
PD1	CLA	4	H3	0.0919	0.0938	0.0927	0.0916
PD2	CLA	5	MG	0.3877	0.3894	0.3742	0.4002
PD2	CLA	5	CHA	0.2201	0.2195	0.2206	0.2376
PD2	CLA	5	CHB	-0.3561	-0.352	-0.3514	-0.3353
PD2	CLA	5	HHB	0.1382	0.1363	0.136	0.1371
PD2	CLA	5	CHC	-0.0512	-0.0825	-0.1208	-0.158
PD2	CLA	5	HHC	0.0725	0.088	0.1086	0.1151
PD2	CLA	5	CHD	-0.3568	-0.3482	-0.3635	-0.3816
PD2	CLA	5	HHD	0.1916	0.1898	0.192	0.1922
PD2	CLA	5	NA	0.063	0.0673	0.0678	0.0901
PD2	CLA	5	C1A	-0.3426	-0.3459	-0.3428	-0.3577
PD2	CLA	5	C2A	0.1162	0.1245	0.1108	0.1587
PD2	CLA	5	H2A	0.0162	0.0159	0.0186	0.0131
PD2	CLA	5	C3A	0.3913	0.3821	0.391	0.3537
PD2	CLA	5	H3A	-0.0523	-0.0492	-0.0523	-0.0385
PD2	CLA	5	C4A	-0.0677	-0.0633	-0.0667	-0.0686
PD2	CLA	5	CMA	-0.4364	-0.439	-0.435	-0.4331
PD2	CLA	5	HMA1	0.0778	0.0785	0.0769	0.0817
PD2	CLA	5	HMA2	0.1015	0.1025	0.1008	0.1001
PD2	CLA	5	HMA3	0.1227	0.1237	0.1226	0.1256
PD2	CLA	5	CAA	0.1195	0.1177	0.1231	0.0946
PD2	CLA	5	HAA1	0.0363	0.0365	0.0348	0.0423
PD2	CLA	5	HAA2	0.0167	0.0175	0.0166	0.0222
PD2	CLA	5	CBA	-0.6297	-0.6331	-0.6303	-0.6266

PD2	CLA	5HBA1	0.1506	0.1512	0.1504	0.1512
PD2	CLA	5HBA2	0.1443	0.145	0.1445	0.1441
PD2	CLA	5 CGA	0.8263	0.8281	0.8273	0.8282
PD2	CLA	5 O1A	-0.5467	-0.547	-0.5473	-0.5444
PD2	CLA	5 O2A	-0.3372	-0.3381	-0.3376	-0.3385
PD2	CLA	5 NB	-0.3104	-0.3252	-0.3174	-0.3278
PD2	CLA	5 C1B	0.1723	0.1742	0.1651	0.1712
PD2	CLA	5 C2B	0.0594	0.066	0.0658	0.0723
PD2	CLA	5 C3B	0.0438	0.0112	0.001	-0.0153
PD2	CLA	5 C4B	-0.0061	0.0261	0.0576	0.0811
PD2	CLA	5 CMB	-0.2969	-0.2844	-0.2793	-0.291
PD2	CLA	5HMB1	0.0666	0.0649	0.0633	0.0701
PD2	CLA	5HMB2	0.0906	0.0874	0.0862	0.0903
PD2	CLA	5HMB3	0.0849	0.0795	0.0794	0.0857
PD2	CLA	5 CAB	-0.1702	-0.1243	-0.1122	-0.0709
PD2	CLA	5 HAB	0.1823	0.1344	0.0936	0.0547
PD2	CLA	5 CBB	-0.3023	-0.3172	-0.3216	-0.3211
PD2	CLA	5HBB1	0.1136	0.1219	0.1314	0.1309
PD2	CLA	5HBB2	0.1508	0.1527	0.1532	0.1553
PD2	CLA	5 NC	-0.2926	-0.2962	-0.2873	-0.3615
PD2	CLA	5 C1C	0.0808	0.0931	0.0965	0.21
PD2	CLA	5 C2C	0.1662	0.17	0.1541	0.0624
PD2	CLA	5 C3C	-0.2428	-0.3044	-0.235	-0.22
PD2	CLA	5 C4C	0.2745	0.2798	0.2795	0.3258
PD2	CLA	5 CMC	-0.4443	-0.4092	-0.4372	-0.3187
PD2	CLA	5HMC1	0.1094	0.0934	0.1064	0.0446
PD2	CLA	5HMC2	0.1195	0.1107	0.1165	0.0955
PD2	CLA	5HMC3	0.1646	0.1589	0.1628	0.1479
PD2	CLA	5 CAC	0.2673	0.3138	0.2618	0.2632
PD2	CLA	5HAC1	0.011	0.007	0.0111	0.0136
PD2	CLA	5HAC2	0.0112	0.0019	0.0128	0.0151
PD2	CLA	5 CBC	-0.4173	-0.4419	-0.4166	-0.4272
PD2	CLA	5HBC1	0.0929	0.0967	0.0933	0.0974
PD2	CLA	5HBC2	0.1357	0.1382	0.1357	0.1421
PD2	CLA	5HBC3	0.0887	0.1005	0.0876	0.0889
PD2	CLA	5 ND	-0.1627	-0.1637	-0.1626	-0.1775

PD2	CLA		5	C1D	0.1117	0.1113	0.1168	0.1565
PD2	CLA		5	C2D	0.1797	0.1777	0.1772	0.1724
PD2	CLA		5	C3D	-0.3487	-0.3467	-0.3474	-0.3414
PD2	CLA		5	C4D	0.0282	0.0303	0.028	0.0278
PD2	CLA		5	CMD	-0.3813	-0.3798	-0.3782	-0.3781
PD2	CLA		5	HMD1	0.1405	0.1404	0.14	0.1453
PD2	CLA		5	HMD2	0.112	0.1119	0.1114	0.1142
PD2	CLA		5	HMD3	0.1523	0.1516	0.1515	0.1538
PD2	CLA		5	CAD	0.7395	0.7395	0.739	0.7417
PD2	CLA		5	OBD	-0.488	-0.4874	-0.4876	-0.4781
PD2	CLA		5	CBD	-0.6856	-0.6894	-0.6871	-0.6935
PD2	CLA		5	HBD1	0.1872	0.1891	0.188	0.1919
PD2	CLA		5	CGD	0.8221	0.8227	0.8232	0.8226
PD2	CLA		5	O1D	-0.5454	-0.5449	-0.5457	-0.5455
PD2	CLA		5	O2D	-0.3573	-0.3577	-0.3582	-0.3575
PD2	CLA		5	CED	-0.1132	-0.109	-0.1116	-0.1113
PD2	CLA		5	HED1	0.1211	0.1199	0.1207	0.1212
PD2	CLA		5	HED2	0.1081	0.1071	0.1077	0.1088
PD2	CLA		5	HED3	0.1199	0.1185	0.1194	0.123
PD2	CLA		5	C1	-0.1032	-0.0992	-0.1045	-0.1048
PD2	CLA		5	H1	0.0828	0.0815	0.0832	0.0849
PD2	CLA		5	H2	0.115	0.1139	0.1158	0.1171
PD2	CLA		5	H3	0.1132	0.1121	0.1136	0.1146
PD1	HIS	A	198	ND1	-0.3188			
PD1	HIS	A	198	HD1	0.4276			
PD1	HIS	A	198	CG	0.2778			
PD1	HIS	A	198	CB	-0.3939			
PD1	HIS	A	198	HB1	0.1894			
PD1	HIS	A	198	HB2	0.1745			
PD1	HIS	A	198	NE2	-0.1072			
PD1	HIS	A	198	CD2	-0.2075			
PD1	HIS	A	198	HD2	0.1457			
PD1	HIS	A	198	CE1	-0.0216			
PD1	HIS	A	198	HE1	0.1605			
PD1	GLN	A	198	CB		-0.2263		
PD1	GLN	A	198	HB1		0.1345		

PD1	GLN	A	198	HB2		0.0775		
PD1	GLN	A	198	CG		-0.0347		
PD1	GLN	A	198	HG1		0.0336		
PD1	GLN	A	198	HG2		0.0866		
PD1	GLN	A	198	CD		0.6406		
PD1	GLN	A	198	OE1		-0.528		
PD1	GLN	A	198	NE2		-0.8182		
PD1	GLN	A	198	HE21		0.4114		
PD1	GLN	A	198	HE22		0.4555		
PD1	HOH		1	O			-0.859	
PD1	HOH		1	H1			0.4228	
PD1	HOH		1	H2			0.4855	
PD1	HOH		2	O			-0.8869	
PD1	HOH		2	H1			0.4942	
PD1	HOH		2	H2			0.4153	
PD1	HOH		86	O			-0.8582	
PD1	HOH		86	H1			0.4486	
PD1	HOH		86	H2			0.4723	
PD2	HIS	D	197	ND1	-0.3536	-0.3683	-0.3447	-0.3536
PD2	HIS	D	197	HD1	0.4221	0.4244	0.4209	0.4235
PD2	HIS	D	197	CG	0.3387	0.348	0.3338	0.3437
PD2	HIS	D	197	CB	-0.3863	-0.3886	-0.3855	-0.3889
PD2	HIS	D	197	HB1	0.1822	0.1819	0.1823	0.1841
PD2	HIS	D	197	HB2	0.1706	0.1714	0.1702	0.1734
PD2	HIS	D	197	NE2	-0.1161	-0.1188	-0.1102	-0.1333
PD2	HIS	D	197	CD2	-0.3092	-0.3154	-0.3063	-0.3044
PD2	HIS	D	197	HD2	0.1671	0.1687	0.1665	0.1654
PD2	HIS	D	197	CE1	0.0622	0.0766	0.0488	0.068
PD2	HIS	D	197	HE1	0.1163	0.1166	0.1214	0.1149
PD1					0.7395	0.7594	0.7735	0.629
PD2					0.2609	0.2409	0.2268	0.371

(c) Atomic coordinates in calculations with axial ligands in MM region.

(c-1) wild type

residue	atom	x	y	z	
CLA	4	MG	-19.914	-45.136	189.572
CLA	4	CHA	-23.352	-44.836	188.885
CLA	4	CHB	-19.556	-46.569	186.476
CLA	4	HHB	-19.428	-47.128	185.559
CLA	4	CHC	-16.545	-44.432	189.617
CLA	4	HHC	-15.478	-44.254	189.665
CLA	4	CHD	-20.349	-42.887	192.209
CLA	4	HHD	-20.478	-42.246	193.076
CLA	4	NA	-21.283	-45.601	187.915
CLA	4	C1A	-22.65	-45.406	187.854
CLA	4	C2A	-23.201	-45.815	186.503
CLA	4	H2A	-24.15	-46.348	186.614
CLA	4	C3A	-22.073	-46.733	185.991
CLA	4	H3A	-21.883	-46.589	184.922
CLA	4	C4A	-20.882	-46.272	186.824
CLA	4	CMA	-22.35	-48.216	186.273
CLA	4	HMA1	-23.241	-48.561	185.738
CLA	4	HMA2	-22.508	-48.382	187.344
CLA	4	HMA3	-21.498	-48.822	185.957
CLA	4	CAA	-23.421	-44.569	185.606
CLA	4	HAA1	-22.443	-44.148	185.355
CLA	4	HAA2	-23.963	-43.802	186.166
CLA	4	CBA	-24.185	-44.844	184.31
CLA	4	HBA1	-23.743	-45.663	183.73
CLA	4	HBA2	-24.137	-43.961	183.661
CLA	4	CGA	-25.652	-45.156	184.538
CLA	4	O1A	-26.229	-45.085	185.603
CLA	4	O2A	-26.251	-45.522	183.387
CLA	4	NB	-18.327	-45.45	188.28
CLA	4	C1B	-18.379	-46.161	187.108
CLA	4	C2B	-17.035	-46.376	186.589
CLA	4	C3B	-16.175	-45.721	187.446
CLA	4	C4B	-17.013	-45.169	188.517
CLA	4	CMB	-16.7	-47.185	185.385
CLA	4	HMB1	-17.547	-47.781	185.038
CLA	4	HMB2	-15.886	-47.877	185.619
CLA	4	HMB3	-16.369	-46.554	184.552
CLA	4	CAB	-14.738	-45.517	187.374
CLA	4	HAB	-14.286	-45.054	188.245
CLA	4	CBB	-13.918	-45.781	186.344
CLA	4	HBB1	-12.865	-45.536	186.408
CLA	4	HBB2	-14.27	-46.173	185.4
CLA	4	NC	-18.661	-43.935	190.761
CLA	4	C1C	-17.298	-43.835	190.626
CLA	4	C2C	-16.749	-42.961	191.654
CLA	4	C3C	-17.809	-42.527	192.406
CLA	4	C4C	-19.007	-43.147	191.82
CLA	4	CMC	-15.301	-42.627	191.827
CLA	4	HMC1	-14.837	-42.345	190.877
CLA	4	HMC2	-14.744	-43.469	192.238

CLA	4 HMC3	-15.159	-41.803	192.524
CLA	4 CAC	-17.715	-41.622	193.598
CLA	4 HAC1	-17.066	-42.12	194.329
CLA	4 HAC2	-18.694	-41.534	194.068
CLA	4 CBC	-17.158	-40.207	193.341
CLA	4 HBC1	-16.245	-40.215	192.743
CLA	4 HBC2	-16.912	-39.738	194.296
CLA	4 HBC3	-17.871	-39.562	192.825
CLA	4 ND	-21.467	-44.114	190.415
CLA	4 C1D	-21.501	-43.294	191.539
CLA	4 C2D	-22.897	-42.907	191.822
CLA	4 C3D	-23.637	-43.51	190.829
CLA	4 C4D	-22.731	-44.239	190.011
CLA	4 CMD	-23.374	-42.105	192.97
CLA	4 HMD1	-22.53	-41.85	193.602
CLA	4 HMD2	-24.094	-42.672	193.568
CLA	4 HMD3	-23.885	-41.187	192.66
CLA	4 CAD	-24.972	-43.554	190.231
CLA	4 OBD	-25.979	-42.96	190.547
CLA	4 CBD	-24.829	-44.466	188.933
CLA	4 HBD1	-25.157	-43.882	188.068
CLA	4 CGD	-25.848	-45.557	189.042
CLA	4 O1D	-25.66	-46.646	189.54
CLA	4 O2D	-27.022	-45.099	188.608
CLA	4 CED	-28.158	-45.94	188.828
CLA	4 HED1	-28.053	-46.468	189.775
CLA	4 HED2	-28.244	-46.665	188.015
CLA	4 HED3	-29.017	-45.269	188.85
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.763	-46.629	184.292
CLA	4 H2	-27.933	-46.264	182.54
CLA	4 H3	-28.233	-44.99	183.765
CLA	5 MG	-13.534	-42.66	185.027
CLA	5 CHA	-10.514	-44.017	183.826
CLA	5 CHB	-15.145	-44.492	182.583
CLA	5 HHB	-15.684	-44.965	181.767
CLA	5 CHC	-16.483	-42.158	186.638
CLA	5 HHC	-17.434	-41.882	187.078
CLA	5 CHD	-11.836	-41.675	187.893
CLA	5 HHD	-11.296	-41.27	188.743
CLA	5 NA	-12.884	-43.982	183.384
CLA	5 C1A	-11.608	-44.346	183.052
CLA	5 C2A	-11.569	-45.224	181.821
CLA	5 H2A	-10.831	-44.849	181.098
CLA	5 C3A	-13.005	-45.08	181.286
CLA	5 H3A	-13.398	-46.061	181.019
CLA	5 C4A	-13.761	-44.494	182.477
CLA	5 CMA	-13.083	-44.142	180.081
CLA	5 HMA1	-12.495	-44.523	179.238
CLA	5 HMA2	-12.707	-43.151	180.354
CLA	5 HMA3	-14.117	-44.033	179.758
CLA	5 CAA	-11.203	-46.676	182.169
CLA	5 HAA1	-11.949	-47.06	182.871
CLA	5 HAA2	-10.241	-46.718	182.683

CLA	5 CBA	-11.139	-47.582	180.932
CLA	5 HBA1	-10.305	-47.264	180.299
CLA	5 HBA2	-12.057	-47.534	180.344
CLA	5 CGA	-10.948	-49.024	181.33
CLA	5 O1A	-11.75	-49.91	181.133
CLA	5 O2A	-9.776	-49.191	181.965
CLA	5 NB	-15.472	-43.261	184.682
CLA	5 C1B	-15.948	-43.965	183.628
CLA	5 C2B	-17.404	-44.078	183.719
CLA	5 C3B	-17.778	-43.399	184.858
CLA	5 C4B	-16.547	-42.901	185.467
CLA	5 CMB	-18.282	-44.844	182.784
CLA	5 HMB1	-17.972	-45.893	182.71
CLA	5 HMB2	-18.276	-44.434	181.767
CLA	5 HMB3	-19.309	-44.819	183.151
CLA	5 CAB	-19.097	-43.183	185.469
CLA	5 HAB	-19.164	-43.428	186.528
CLA	5 CBB	-20.172	-42.65	184.876
CLA	5 HBB1	-21.087	-42.466	185.428
CLA	5 HBB2	-20.157	-42.321	183.845
CLA	5 NC	-14.068	-42.065	186.974
CLA	5 C1C	-15.33	-41.721	187.331
CLA	5 C2C	-15.31	-40.844	188.496
CLA	5 C3C	-13.987	-40.685	188.84
CLA	5 C4C	-13.222	-41.48	187.887
CLA	5 CMC	-16.511	-40.231	189.141
CLA	5 HMC1	-17.044	-40.965	189.757
CLA	5 HMC2	-17.213	-39.835	188.399
CLA	5 HMC3	-16.237	-39.406	189.802
CLA	5 CAC	-13.421	-39.779	189.895
CLA	5 HAC1	-12.967	-40.358	190.707
CLA	5 HAC2	-14.244	-39.226	190.357
CLA	5 CBC	-12.39	-38.777	189.336
CLA	5 HBC1	-11.372	-39.166	189.425
CLA	5 HBC2	-12.427	-37.833	189.879
CLA	5 HBC3	-12.591	-38.554	188.283
CLA	5 ND	-11.632	-42.845	185.757
CLA	5 C1D	-11.075	-42.359	186.929
CLA	5 C2D	-9.636	-42.609	186.941
CLA	5 C3D	-9.37	-43.204	185.723
CLA	5 C4D	-10.612	-43.346	185.052
CLA	5 CMD	-8.68	-42.299	188.027
CLA	5 HMD1	-8.634	-43.092	188.78
CLA	5 HMD2	-9.006	-41.399	188.533
CLA	5 HMD3	-7.67	-42.155	187.641
CLA	5 CAD	-8.31	-43.768	184.901
CLA	5 OBD	-7.116	-43.84	185.103
CLA	5 CBD	-9.036	-44.334	183.601
CLA	5 HBD1	-8.806	-45.398	183.509
CLA	5 CGD	-8.453	-43.607	182.414
CLA	5 O1D	-8.618	-42.423	182.235
CLA	5 O2D	-7.711	-44.394	181.632
CLA	5 CED	-6.933	-43.722	180.616
CLA	5 HED1	-6.681	-42.715	180.935

CLA	5 HED2	-7.494	-43.671	179.686
CLA	5 HED3	-6.037	-44.318	180.474
CLA	5 C1	-9.498	-50.523	182.417
CLA	5 H1	-9.685	-51.247	181.623
CLA	5 H2	-10.114	-50.757	183.286
CLA	5 H3	-8.446	-50.527	182.698

(c-2) D1-H198Q.

residue	atom	x	y	z
CLA	4 MG	-19.949	-44.864	189.357
CLA	4 CHA	-23.389	-44.777	188.83
CLA	4 CHB	-19.604	-46.497	186.385
CLA	4 HHB	-19.481	-47.095	185.492
CLA	4 CHC	-16.577	-44.358	189.507
CLA	4 HHC	-15.506	-44.213	189.565
CLA	4 CHD	-20.375	-42.859	192.158
CLA	4 HHD	-20.492	-42.275	193.064
CLA	4 NA	-21.318	-45.475	187.803
CLA	4 C1A	-22.692	-45.322	187.783
CLA	4 C2A	-23.253	-45.747	186.443
CLA	4 H2A	-24.208	-46.267	186.556
CLA	4 C3A	-22.131	-46.679	185.936
CLA	4 H3A	-21.962	-46.568	184.86
CLA	4 C4A	-20.928	-46.184	186.731
CLA	4 CMA	-22.4	-48.156	186.268
CLA	4 HMA1	-23.29	-48.522	185.744
CLA	4 HMA2	-22.562	-48.286	187.344
CLA	4 HMA3	-21.548	-48.773	185.975
CLA	4 CAA	-23.449	-44.491	185.555
CLA	4 HAA1	-22.463	-44.082	185.312
CLA	4 HAA2	-23.981	-43.723	186.122
CLA	4 CBA	-24.215	-44.736	184.257
CLA	4 HBA1	-23.774	-45.535	183.651
CLA	4 HBA2	-24.179	-43.832	183.636
CLA	4 CGA	-25.676	-45.058	184.494
CLA	4 O1A	-26.261	-44.935	185.55
CLA	4 O2A	-26.261	-45.501	183.364
CLA	4 NB	-18.364	-45.326	188.143
CLA	4 C1B	-18.422	-46.09	187.007
CLA	4 C2B	-17.077	-46.368	186.523
CLA	4 C3B	-16.21	-45.713	187.374
CLA	4 C4B	-17.048	-45.091	188.405
CLA	4 CMB	-16.749	-47.237	185.36
CLA	4 HMB1	-17.585	-47.883	185.082
CLA	4 HMB2	-15.9	-47.881	185.607
CLA	4 HMB3	-16.473	-46.649	184.477
CLA	4 CAB	-14.765	-45.575	187.325
CLA	4 HAB	-14.298	-45.188	188.225
CLA	4 CBB	-13.957	-45.81	186.28
CLA	4 HBB1	-12.892	-45.629	186.357
CLA	4 HBB2	-14.329	-46.121	185.312
CLA	4 NC	-18.693	-43.819	190.631
CLA	4 C1C	-17.324	-43.768	190.528
CLA	4 C2C	-16.769	-42.996	191.627
CLA	4 C3C	-17.832	-42.582	192.392
CLA	4 C4C	-19.035	-43.112	191.748
CLA	4 CMC	-15.318	-42.728	191.867
CLA	4 HMC1	-15.031	-41.719	191.556
CLA	4 HMC2	-14.695	-43.424	191.306
CLA	4 HMC3	-15.071	-42.826	192.928

CLA	4 CAC	-17.739	-41.775	193.646
CLA	4 HAC1	-17.15	-42.362	194.364
CLA	4 HAC2	-18.734	-41.658	194.077
CLA	4 CBC	-17.091	-40.386	193.503
CLA	4 HBC1	-16.107	-40.438	193.033
CLA	4 HBC2	-16.952	-39.95	194.494
CLA	4 HBC3	-17.711	-39.703	192.915
CLA	4 ND	-21.504	-43.987	190.317
CLA	4 C1D	-21.535	-43.23	191.482
CLA	4 C2D	-22.935	-42.899	191.808
CLA	4 C3D	-23.679	-43.499	190.813
CLA	4 C4D	-22.769	-44.17	189.952
CLA	4 CMD	-23.404	-42.126	192.98
CLA	4 HMD1	-22.553	-41.875	193.605
CLA	4 HMD2	-24.113	-42.706	193.577
CLA	4 HMD3	-23.92	-41.204	192.692
CLA	4 CAD	-25.016	-43.547	190.22
CLA	4 OBD	-26.022	-42.957	190.541
CLA	4 CBD	-24.873	-44.442	188.908
CLA	4 HBD1	-25.224	-43.85	188.057
CLA	4 CGD	-25.87	-45.551	189.021
CLA	4 O1D	-25.665	-46.637	189.521
CLA	4 O2D	-27.053	-45.109	188.593
CLA	4 CED	-28.18	-45.954	188.838
CLA	4 HED1	-28.054	-46.478	189.785
CLA	4 HED2	-28.279	-46.684	188.031
CLA	4 HED3	-29.042	-45.288	188.874
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.741	-46.621	184.304
CLA	4 H2	-27.94	-46.283	182.55
CLA	4 H3	-28.246	-44.998	183.762
CLA	5 MG	-13.534	-42.664	185.02
CLA	5 CHA	-10.513	-44.019	183.824
CLA	5 CHB	-15.141	-44.492	182.569
CLA	5 HHB	-15.679	-44.961	181.75
CLA	5 CHC	-16.484	-42.15	186.616
CLA	5 HHC	-17.434	-41.865	187.051
CLA	5 CHD	-11.84	-41.676	187.887
CLA	5 HHD	-11.3	-41.268	188.736
CLA	5 NA	-12.882	-43.984	183.376
CLA	5 C1A	-11.607	-44.348	183.047
CLA	5 C2A	-11.564	-45.225	181.816
CLA	5 H2A	-10.823	-44.853	181.097
CLA	5 C3A	-12.998	-45.08	181.277
CLA	5 H3A	-13.391	-46.061	181.008
CLA	5 C4A	-13.758	-44.494	182.465
CLA	5 CMA	-13.071	-44.143	180.07
CLA	5 HMA1	-12.477	-44.522	179.232
CLA	5 HMA2	-12.698	-43.15	180.347
CLA	5 HMA3	-14.102	-44.035	179.74
CLA	5 CAA	-11.204	-46.678	182.166
CLA	5 HAA1	-11.953	-47.061	182.865
CLA	5 HAA2	-10.243	-46.723	182.684
CLA	5 CBA	-11.137	-47.583	180.929

CLA	5 HBA1	-10.301	-47.265	180.298
CLA	5 HBA2	-12.053	-47.535	180.338
CLA	5 CGA	-10.947	-49.025	181.328
CLA	5 O1A	-11.75	-49.911	181.132
CLA	5 O2A	-9.775	-49.192	181.963
CLA	5 NB	-15.471	-43.265	184.669
CLA	5 C1B	-15.947	-43.964	183.612
CLA	5 C2B	-17.403	-44.064	183.693
CLA	5 C3B	-17.78	-43.378	184.827
CLA	5 C4B	-16.547	-42.893	185.445
CLA	5 CMB	-18.284	-44.818	182.751
CLA	5 HMB1	-17.987	-45.871	182.676
CLA	5 HMB2	-18.266	-44.407	181.735
CLA	5 HMB3	-19.312	-44.781	183.111
CLA	5 CAB	-19.098	-43.145	185.431
CLA	5 HAB	-19.163	-43.374	186.493
CLA	5 CBB	-20.175	-42.618	184.837
CLA	5 HBB1	-21.087	-42.428	185.392
CLA	5 HBB2	-20.168	-42.301	183.803
CLA	5 NC	-14.07	-42.071	186.966
CLA	5 C1C	-15.331	-41.722	187.317
CLA	5 C2C	-15.314	-40.845	188.484
CLA	5 C3C	-13.993	-40.69	188.833
CLA	5 C4C	-13.225	-41.486	187.881
CLA	5 CMC	-16.516	-40.231	189.127
CLA	5 HMC1	-17.054	-40.968	189.732
CLA	5 HMC2	-17.212	-39.827	188.384
CLA	5 HMC3	-16.242	-39.412	189.794
CLA	5 CAC	-13.427	-39.789	189.892
CLA	5 HAC1	-12.97	-40.373	190.699
CLA	5 HAC2	-14.249	-39.239	190.357
CLA	5 CBC	-12.395	-38.783	189.338
CLA	5 HBC1	-11.377	-39.17	189.429
CLA	5 HBC2	-12.437	-37.841	189.882
CLA	5 HBC3	-12.594	-38.559	188.285
CLA	5 ND	-11.634	-42.847	185.752
CLA	5 C1D	-11.078	-42.36	186.924
CLA	5 C2D	-9.637	-42.609	186.937
CLA	5 C3D	-9.371	-43.204	185.72
CLA	5 C4D	-10.612	-43.348	185.048
CLA	5 CMD	-8.683	-42.297	188.024
CLA	5 HMD1	-8.637	-43.09	188.777
CLA	5 HMD2	-9.01	-41.397	188.529
CLA	5 HMD3	-7.673	-42.153	187.639
CLA	5 CAD	-8.31	-43.769	184.899
CLA	5 OBD	-7.116	-43.839	185.102
CLA	5 CBD	-9.035	-44.334	183.598
CLA	5 HBD1	-8.804	-45.398	183.506
CLA	5 CGD	-8.452	-43.606	182.412
CLA	5 O1D	-8.619	-42.422	182.234
CLA	5 O2D	-7.71	-44.392	181.631
CLA	5 CED	-6.929	-43.722	180.615
CLA	5 HED1	-6.674	-42.716	180.937
CLA	5 HED2	-7.49	-43.667	179.686

CLA	5	HED3	-6.036	-44.32	180.473
CLA	5	C1	-9.498	-50.523	182.417
CLA	5	H1	-9.684	-51.248	181.624
CLA	5	H2	-10.115	-50.756	183.285
CLA	5	H3	-8.446	-50.527	182.7

(c-3) D1-H198A + H_2O.

residue	atom	x	y	z
CLA	4 MG	-19.951	-45.145	189.613
CLA	4 CHA	-23.372	-44.813	188.892
CLA	4 CHB	-19.581	-46.583	186.505
CLA	4 HHB	-19.453	-47.14	185.586
CLA	4 CHC	-16.58	-44.428	189.638
CLA	4 HHC	-15.512	-44.253	189.683
CLA	4 CHD	-20.378	-42.842	192.214
CLA	4 HHD	-20.506	-42.207	193.085
CLA	4 NA	-21.305	-45.59	187.927
CLA	4 C1A	-22.672	-45.389	187.864
CLA	4 C2A	-23.224	-45.801	186.514
CLA	4 H2A	-24.175	-46.329	186.625
CLA	4 C3A	-22.098	-46.723	186.003
CLA	4 H3A	-21.901	-46.572	184.936
CLA	4 C4A	-20.91	-46.271	186.845
CLA	4 CMA	-22.385	-48.208	186.268
CLA	4 HMA1	-23.271	-48.544	185.718
CLA	4 HMA2	-22.559	-48.383	187.335
CLA	4 HMA3	-21.533	-48.815	185.955
CLA	4 CAA	-23.436	-44.553	185.617
CLA	4 HAA1	-22.455	-44.135	185.371
CLA	4 HAA2	-23.978	-43.785	186.174
CLA	4 CBA	-24.194	-44.823	184.316
CLA	4 HBA1	-23.75	-45.641	183.735
CLA	4 HBA2	-24.142	-43.938	183.671
CLA	4 CGA	-25.662	-45.133	184.538
CLA	4 O1A	-26.247	-45.046	185.598
CLA	4 O2A	-26.252	-45.518	183.389
CLA	4 NB	-18.359	-45.477	188.321
CLA	4 C1B	-18.409	-46.178	187.14
CLA	4 C2B	-17.063	-46.378	186.613
CLA	4 C3B	-16.208	-45.718	187.47
CLA	4 C4B	-17.051	-45.18	188.547
CLA	4 CMB	-16.723	-47.172	185.4
CLA	4 HMB1	-17.567	-47.768	185.046
CLA	4 HMB2	-15.906	-47.863	185.626
CLA	4 HMB3	-16.395	-46.53	184.574
CLA	4 CAB	-14.773	-45.498	187.395
CLA	4 HAB	-14.326	-45.021	188.261
CLA	4 CBB	-13.948	-45.768	186.371
CLA	4 HBB1	-12.897	-45.512	186.435
CLA	4 HBB2	-14.292	-46.176	185.43
CLA	4 NC	-18.693	-43.9	190.77
CLA	4 C1C	-17.327	-43.814	190.638
CLA	4 C2C	-16.77	-42.94	191.662
CLA	4 C3C	-17.826	-42.494	192.41
CLA	4 C4C	-19.032	-43.106	191.824
CLA	4 CMC	-15.318	-42.621	191.834
CLA	4 HMC1	-14.844	-42.379	190.878
CLA	4 HMC2	-14.775	-43.457	192.278
CLA	4 HMC3	-15.168	-41.775	192.501

CLA	4 CAC	-17.718	-41.586	193.599
CLA	4 HAC1	-17.062	-42.083	194.324
CLA	4 HAC2	-18.692	-41.495	194.079
CLA	4 CBC	-17.158	-40.173	193.331
CLA	4 HBC1	-16.258	-40.188	192.714
CLA	4 HBC2	-16.89	-39.705	194.28
CLA	4 HBC3	-17.878	-39.525	192.828
CLA	4 ND	-21.491	-44.058	190.411
CLA	4 C1D	-21.53	-43.244	191.539
CLA	4 C2D	-22.932	-42.876	191.828
CLA	4 C3D	-23.667	-43.485	190.835
CLA	4 C4D	-22.753	-44.204	190.014
CLA	4 CMD	-23.415	-42.081	192.976
CLA	4 HMD1	-22.572	-41.838	193.614
CLA	4 HMD2	-24.145	-42.645	193.564
CLA	4 HMD3	-23.912	-41.155	192.669
CLA	4 CAD	-25	-43.537	190.235
CLA	4 OBD	-26.009	-42.945	190.549
CLA	4 CBD	-24.851	-44.45	188.939
CLA	4 HBD1	-25.181	-43.867	188.075
CLA	4 CGD	-25.865	-45.546	189.041
CLA	4 O1D	-25.674	-46.641	189.525
CLA	4 O2D	-27.042	-45.085	188.616
CLA	4 CED	-28.174	-45.933	188.832
CLA	4 HED1	-28.067	-46.463	189.778
CLA	4 HED2	-28.256	-46.657	188.018
CLA	4 HED3	-29.036	-45.266	188.856
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.763	-46.611	184.309
CLA	4 H2	-27.924	-46.29	182.548
CLA	4 H3	-28.241	-44.988	183.74
CLA	5 MG	-13.534	-42.661	185.031
CLA	5 CHA	-10.514	-44.016	183.827
CLA	5 CHB	-15.146	-44.491	182.587
CLA	5 HHB	-15.684	-44.963	181.771
CLA	5 CHC	-16.483	-42.155	186.642
CLA	5 HHC	-17.434	-41.877	187.08
CLA	5 CHD	-11.835	-41.674	187.896
CLA	5 HHD	-11.295	-41.269	188.745
CLA	5 NA	-12.885	-43.985	183.389
CLA	5 C1A	-11.607	-44.346	183.055
CLA	5 C2A	-11.569	-45.223	181.823
CLA	5 H2A	-10.833	-44.849	181.098
CLA	5 C3A	-13.006	-45.08	181.29
CLA	5 H3A	-13.4	-46.061	181.023
CLA	5 C4A	-13.761	-44.494	182.482
CLA	5 CMA	-13.087	-44.142	180.085
CLA	5 HMA1	-12.501	-44.523	179.241
CLA	5 HMA2	-12.709	-43.151	180.358
CLA	5 HMA3	-14.121	-44.032	179.764
CLA	5 CAA	-11.203	-46.675	182.171
CLA	5 HAA1	-11.947	-47.059	182.875
CLA	5 HAA2	-10.239	-46.717	182.682
CLA	5 CBA	-11.143	-47.582	180.934

CLA	5 HBA1	-10.31	-47.265	180.298
CLA	5 HBA2	-12.062	-47.535	180.348
CLA	5 CGA	-10.951	-49.024	181.332
CLA	5 O1A	-11.753	-49.911	181.138
CLA	5 O2A	-9.777	-49.192	181.965
CLA	5 NB	-15.473	-43.261	184.686
CLA	5 C1B	-15.949	-43.964	183.632
CLA	5 C2B	-17.404	-44.076	183.722
CLA	5 C3B	-17.778	-43.397	184.862
CLA	5 C4B	-16.547	-42.9	185.47
CLA	5 CMB	-18.283	-44.842	182.788
CLA	5 HMB1	-17.974	-45.891	182.713
CLA	5 HMB2	-18.277	-44.432	181.771
CLA	5 HMB3	-19.31	-44.815	183.154
CLA	5 CAB	-19.097	-43.182	185.473
CLA	5 HAB	-19.166	-43.429	186.532
CLA	5 CBB	-20.172	-42.65	184.88
CLA	5 HBB1	-21.088	-42.467	185.432
CLA	5 HBB2	-20.158	-42.319	183.849
CLA	5 NC	-14.068	-42.065	186.979
CLA	5 C1C	-15.33	-41.719	187.334
CLA	5 C2C	-15.31	-40.841	188.497
CLA	5 C3C	-13.986	-40.684	188.842
CLA	5 C4C	-13.221	-41.48	187.89
CLA	5 CMC	-16.51	-40.222	189.14
CLA	5 HMC1	-17.045	-40.951	189.758
CLA	5 HMC2	-17.21	-39.828	188.395
CLA	5 HMC3	-16.234	-39.395	189.797
CLA	5 CAC	-13.42	-39.776	189.896
CLA	5 HAC1	-12.966	-40.353	190.709
CLA	5 HAC2	-14.243	-39.221	190.356
CLA	5 CBC	-12.388	-38.775	189.336
CLA	5 HBC1	-11.371	-39.166	189.424
CLA	5 HBC2	-12.423	-37.831	189.879
CLA	5 HBC3	-12.59	-38.553	188.283
CLA	5 ND	-11.632	-42.846	185.76
CLA	5 C1D	-11.073	-42.358	186.933
CLA	5 C2D	-9.636	-42.607	186.943
CLA	5 C3D	-9.37	-43.202	185.725
CLA	5 C4D	-10.612	-43.345	185.055
CLA	5 CMD	-8.678	-42.297	188.028
CLA	5 HMD1	-8.629	-43.091	188.78
CLA	5 HMD2	-9.005	-41.398	188.535
CLA	5 HMD3	-7.67	-42.15	187.64
CLA	5 CAD	-8.31	-43.765	184.903
CLA	5 OBD	-7.116	-43.838	185.105
CLA	5 CBD	-9.036	-44.33	183.602
CLA	5 HBD1	-8.806	-45.395	183.51
CLA	5 CGD	-8.452	-43.606	182.414
CLA	5 O1D	-8.615	-42.421	182.233
CLA	5 O2D	-7.713	-44.396	181.633
CLA	5 CED	-6.932	-43.727	180.616
CLA	5 HED1	-6.673	-42.723	180.938
CLA	5 HED2	-7.495	-43.67	179.688

CLA	5 HED3	-6.041	-44.328	180.472
CLA	5 C1	-9.498	-50.523	182.417
CLA	5 H1	-9.687	-51.248	181.625
CLA	5 H2	-10.112	-50.756	183.288
CLA	5 H3	-8.445	-50.527	182.697

(c-4) D1-H198A – H_2O.

residue	atom	x	y	z
CLA	4 MG	-19.893	-44.923	189.403
CLA	4 CHA	-23.345	-44.871	188.89
CLA	4 CHB	-19.552	-46.56	186.433
CLA	4 HHB	-19.425	-47.113	185.513
CLA	4 CHC	-16.527	-44.428	189.57
CLA	4 HHC	-15.46	-44.255	189.617
CLA	4 CHD	-20.327	-42.916	192.197
CLA	4 HHD	-20.456	-42.271	193.059
CLA	4 NA	-21.27	-45.609	187.898
CLA	4 C1A	-22.641	-45.425	187.85
CLA	4 C2A	-23.197	-45.827	186.5
CLA	4 H2A	-24.145	-46.361	186.612
CLA	4 C3A	-22.07	-46.741	185.977
CLA	4 H3A	-21.893	-46.596	184.906
CLA	4 C4A	-20.872	-46.276	186.794
CLA	4 CMA	-22.34	-48.225	186.262
CLA	4 HMA1	-23.233	-48.573	185.733
CLA	4 HMA2	-22.491	-48.393	187.333
CLA	4 HMA3	-21.488	-48.827	185.939
CLA	4 CAA	-23.42	-44.576	185.61
CLA	4 HAA1	-22.442	-44.153	185.358
CLA	4 HAA2	-23.962	-43.812	186.174
CLA	4 CBA	-24.185	-44.845	184.313
CLA	4 HBA1	-23.742	-45.659	183.727
CLA	4 HBA2	-24.14	-43.958	183.669
CLA	4 CGA	-25.651	-45.16	184.541
CLA	4 O1A	-26.226	-45.097	185.609
CLA	4 O2A	-26.251	-45.52	183.389
CLA	4 NB	-18.314	-45.451	188.239
CLA	4 C1B	-18.37	-46.16	187.069
CLA	4 C2B	-17.03	-46.384	186.554
CLA	4 C3B	-16.164	-45.731	187.411
CLA	4 C4B	-16.994	-45.173	188.48
CLA	4 CMB	-16.701	-47.211	185.361
CLA	4 HMB1	-17.545	-47.828	185.042
CLA	4 HMB2	-15.875	-47.884	185.6
CLA	4 HMB3	-16.394	-46.594	184.508
CLA	4 CAB	-14.726	-45.542	187.336
CLA	4 HAB	-14.262	-45.12	188.221
CLA	4 CBB	-13.921	-45.775	186.288
CLA	4 HBB1	-12.863	-45.552	186.351
CLA	4 HBB2	-14.288	-46.127	185.333
CLA	4 NC	-18.642	-43.93	190.717
CLA	4 C1C	-17.278	-43.832	190.587
CLA	4 C2C	-16.731	-42.974	191.624
CLA	4 C3C	-17.793	-42.551	192.386
CLA	4 C4C	-18.988	-43.16	191.797
CLA	4 CMC	-15.282	-42.646	191.802
CLA	4 HMC1	-14.79	-42.465	190.842
CLA	4 HMC2	-14.75	-43.451	192.311
CLA	4 HMC3	-15.143	-41.758	192.416

CLA	4 CAC	-17.708	-41.669	193.597
CLA	4 HAC1	-17.064	-42.181	194.323
CLA	4 HAC2	-18.691	-41.592	194.061
CLA	4 CBC	-17.157	-40.246	193.374
CLA	4 HBC1	-16.234	-40.234	192.792
CLA	4 HBC2	-16.932	-39.793	194.341
CLA	4 HBC3	-17.869	-39.599	192.857
CLA	4 ND	-21.456	-44.191	190.436
CLA	4 C1D	-21.482	-43.345	191.545
CLA	4 C2D	-22.871	-42.945	191.824
CLA	4 C3D	-23.618	-43.548	190.835
CLA	4 C4D	-22.724	-44.298	190.025
CLA	4 CMD	-23.345	-42.133	192.968
CLA	4 HMD1	-22.501	-41.869	193.597
CLA	4 HMD2	-24.058	-42.701	193.574
CLA	4 HMD3	-23.864	-41.222	192.654
CLA	4 CAD	-24.952	-43.57	190.231
CLA	4 OBD	-25.95	-42.961	190.547
CLA	4 CBD	-24.819	-44.481	188.933
CLA	4 HBD1	-25.134	-43.892	188.068
CLA	4 CGD	-25.857	-45.555	189.04
CLA	4 O1D	-25.688	-46.648	189.535
CLA	4 O2D	-27.025	-45.076	188.611
CLA	4 CED	-28.169	-45.909	188.827
CLA	4 HED1	-28.075	-46.437	189.775
CLA	4 HED2	-28.256	-46.637	188.016
CLA	4 HED3	-29.023	-45.231	188.842
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.762	-46.638	184.283
CLA	4 H2	-27.935	-46.252	182.537
CLA	4 H3	-28.233	-44.993	183.777
CLA	5 MG	-13.534	-42.667	185.022
CLA	5 CHA	-10.512	-44.022	183.826
CLA	5 CHB	-15.142	-44.488	182.569
CLA	5 HHB	-15.68	-44.958	181.752
CLA	5 CHC	-16.484	-42.162	186.626
CLA	5 HHC	-17.434	-41.883	187.064
CLA	5 CHD	-11.838	-41.677	187.887
CLA	5 HHD	-11.298	-41.269	188.735
CLA	5 NA	-12.881	-43.982	183.376
CLA	5 C1A	-11.609	-44.35	183.048
CLA	5 C2A	-11.566	-45.226	181.817
CLA	5 H2A	-10.824	-44.852	181.099
CLA	5 C3A	-13.001	-45.079	181.277
CLA	5 H3A	-13.395	-46.06	181.01
CLA	5 C4A	-13.759	-44.492	182.465
CLA	5 CMA	-13.072	-44.143	180.069
CLA	5 HMA1	-12.479	-44.526	179.231
CLA	5 HMA2	-12.697	-43.151	180.344
CLA	5 HMA3	-14.103	-44.034	179.739
CLA	5 CAA	-11.205	-46.679	182.166
CLA	5 HAA1	-11.954	-47.062	182.865
CLA	5 HAA2	-10.245	-46.724	182.683
CLA	5 CBA	-11.139	-47.583	180.929

CLA	5 HBA1	-10.303	-47.266	180.297
CLA	5 HBA2	-12.055	-47.536	180.339
CLA	5 CGA	-10.948	-49.026	181.328
CLA	5 O1A	-11.752	-49.91	181.133
CLA	5 O2A	-9.776	-49.191	181.963
CLA	5 NB	-15.471	-43.267	184.673
CLA	5 C1B	-15.946	-43.965	183.616
CLA	5 C2B	-17.403	-44.075	183.702
CLA	5 C3B	-17.779	-43.397	184.84
CLA	5 C4B	-16.546	-42.905	185.455
CLA	5 CMB	-18.281	-44.834	182.762
CLA	5 HMB1	-17.976	-45.885	182.688
CLA	5 HMB2	-18.267	-44.422	181.746
CLA	5 HMB3	-19.309	-44.804	183.123
CLA	5 CAB	-19.098	-43.177	185.447
CLA	5 HAB	-19.165	-43.425	186.505
CLA	5 CBB	-20.173	-42.641	184.857
CLA	5 HBB1	-21.089	-42.459	185.409
CLA	5 HBB2	-20.161	-42.309	183.826
CLA	5 NC	-14.069	-42.074	186.968
CLA	5 C1C	-15.33	-41.729	187.323
CLA	5 C2C	-15.312	-40.848	188.488
CLA	5 C3C	-13.991	-40.69	188.834
CLA	5 C4C	-13.224	-41.486	187.881
CLA	5 CMC	-16.514	-40.236	189.132
CLA	5 HMC1	-17.04	-40.967	189.756
CLA	5 HMC2	-17.218	-39.849	188.388
CLA	5 HMC3	-16.24	-39.404	189.785
CLA	5 CAC	-13.425	-39.785	189.89
CLA	5 HAC1	-12.97	-40.366	190.7
CLA	5 HAC2	-14.247	-39.233	190.353
CLA	5 CBC	-12.393	-38.781	189.333
CLA	5 HBC1	-11.375	-39.169	189.425
CLA	5 HBC2	-12.434	-37.838	189.877
CLA	5 HBC3	-12.592	-38.558	188.28
CLA	5 ND	-11.634	-42.85	185.754
CLA	5 C1D	-11.078	-42.362	186.923
CLA	5 C2D	-9.635	-42.611	186.937
CLA	5 C3D	-9.37	-43.21	185.722
CLA	5 C4D	-10.612	-43.352	185.049
CLA	5 CMD	-8.681	-42.296	188.024
CLA	5 HMD1	-8.639	-43.085	188.78
CLA	5 HMD2	-9.005	-41.392	188.524
CLA	5 HMD3	-7.67	-42.156	187.639
CLA	5 CAD	-8.31	-43.781	184.902
CLA	5 OBD	-7.118	-43.859	185.11
CLA	5 CBD	-9.036	-44.339	183.599
CLA	5 HBD1	-8.809	-45.404	183.502
CLA	5 CGD	-8.452	-43.606	182.415
CLA	5 O1D	-8.61	-42.418	182.251
CLA	5 O2D	-7.721	-44.39	181.624
CLA	5 CED	-6.936	-43.718	180.612
CLA	5 HED1	-6.674	-42.716	180.94
CLA	5 HED2	-7.498	-43.654	179.684

CLA	5	HED3	-6.047	-44.322	180.466
CLA	5	C1	-9.498	-50.523	182.417
CLA	5	H1	-9.685	-51.249	181.625
CLA	5	H2	-10.113	-50.754	183.287
CLA	5	H3	-8.446	-50.527	182.698

(c-5) D1-H198A + OH^-.

residue	atom	x	y	z
CLA	4 MG	-19.893	-44.923	189.403
CLA	4 CHA	-23.345	-44.871	188.89
CLA	4 CHB	-19.552	-46.56	186.433
CLA	4 HHB	-19.425	-47.113	185.513
CLA	4 CHC	-16.527	-44.428	189.57
CLA	4 HHC	-15.46	-44.255	189.617
CLA	4 CHD	-20.327	-42.916	192.197
CLA	4 HHD	-20.456	-42.271	193.059
CLA	4 NA	-21.27	-45.609	187.898
CLA	4 C1A	-22.641	-45.425	187.85
CLA	4 C2A	-23.197	-45.827	186.5
CLA	4 H2A	-24.145	-46.361	186.612
CLA	4 C3A	-22.07	-46.741	185.977
CLA	4 H3A	-21.893	-46.596	184.906
CLA	4 C4A	-20.872	-46.276	186.794
CLA	4 CMA	-22.34	-48.225	186.262
CLA	4 HMA1	-23.233	-48.573	185.733
CLA	4 HMA2	-22.491	-48.393	187.333
CLA	4 HMA3	-21.488	-48.827	185.939
CLA	4 CAA	-23.42	-44.576	185.61
CLA	4 HAA1	-22.442	-44.153	185.358
CLA	4 HAA2	-23.962	-43.812	186.174
CLA	4 CBA	-24.185	-44.845	184.313
CLA	4 HBA1	-23.742	-45.659	183.727
CLA	4 HBA2	-24.14	-43.958	183.669
CLA	4 CGA	-25.651	-45.16	184.541
CLA	4 O1A	-26.226	-45.097	185.609
CLA	4 O2A	-26.251	-45.52	183.389
CLA	4 NB	-18.314	-45.451	188.239
CLA	4 C1B	-18.37	-46.16	187.069
CLA	4 C2B	-17.03	-46.384	186.554
CLA	4 C3B	-16.164	-45.731	187.411
CLA	4 C4B	-16.994	-45.173	188.48
CLA	4 CMB	-16.701	-47.211	185.361
CLA	4 HMB1	-17.545	-47.828	185.042
CLA	4 HMB2	-15.875	-47.884	185.6
CLA	4 HMB3	-16.394	-46.594	184.508
CLA	4 CAB	-14.726	-45.542	187.336
CLA	4 HAB	-14.262	-45.12	188.221
CLA	4 CBB	-13.921	-45.775	186.288
CLA	4 HBB1	-12.863	-45.552	186.351
CLA	4 HBB2	-14.288	-46.127	185.333
CLA	4 NC	-18.642	-43.93	190.717
CLA	4 C1C	-17.278	-43.832	190.587
CLA	4 C2C	-16.731	-42.974	191.624
CLA	4 C3C	-17.793	-42.551	192.386
CLA	4 C4C	-18.988	-43.16	191.797
CLA	4 CMC	-15.282	-42.646	191.802
CLA	4 HMC1	-14.79	-42.465	190.842
CLA	4 HMC2	-14.75	-43.451	192.311
CLA	4 HMC3	-15.143	-41.758	192.416

CLA	4 CAC	-17.708	-41.669	193.597
CLA	4 HAC1	-17.064	-42.181	194.323
CLA	4 HAC2	-18.691	-41.592	194.061
CLA	4 CBC	-17.157	-40.246	193.374
CLA	4 HBC1	-16.234	-40.234	192.792
CLA	4 HBC2	-16.932	-39.793	194.341
CLA	4 HBC3	-17.869	-39.599	192.857
CLA	4 ND	-21.456	-44.191	190.436
CLA	4 C1D	-21.482	-43.345	191.545
CLA	4 C2D	-22.871	-42.945	191.824
CLA	4 C3D	-23.618	-43.548	190.835
CLA	4 C4D	-22.724	-44.298	190.025
CLA	4 CMD	-23.345	-42.133	192.968
CLA	4 HMD1	-22.501	-41.869	193.597
CLA	4 HMD2	-24.058	-42.701	193.574
CLA	4 HMD3	-23.864	-41.222	192.654
CLA	4 CAD	-24.952	-43.57	190.231
CLA	4 OBD	-25.95	-42.961	190.547
CLA	4 CBD	-24.819	-44.481	188.933
CLA	4 HBD1	-25.134	-43.892	188.068
CLA	4 CGD	-25.857	-45.555	189.04
CLA	4 O1D	-25.688	-46.648	189.535
CLA	4 O2D	-27.025	-45.076	188.611
CLA	4 CED	-28.169	-45.909	188.827
CLA	4 HED1	-28.075	-46.437	189.775
CLA	4 HED2	-28.256	-46.637	188.016
CLA	4 HED3	-29.023	-45.231	188.842
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.762	-46.638	184.283
CLA	4 H2	-27.935	-46.252	182.537
CLA	4 H3	-28.233	-44.993	183.777
CLA	5 MG	-13.534	-42.667	185.022
CLA	5 CHA	-10.512	-44.022	183.826
CLA	5 CHB	-15.142	-44.488	182.569
CLA	5 HHB	-15.68	-44.958	181.752
CLA	5 CHC	-16.484	-42.162	186.626
CLA	5 HHC	-17.434	-41.883	187.064
CLA	5 CHD	-11.838	-41.677	187.887
CLA	5 HHD	-11.298	-41.269	188.735
CLA	5 NA	-12.881	-43.982	183.376
CLA	5 C1A	-11.609	-44.35	183.048
CLA	5 C2A	-11.566	-45.226	181.817
CLA	5 H2A	-10.824	-44.852	181.099
CLA	5 C3A	-13.001	-45.079	181.277
CLA	5 H3A	-13.395	-46.06	181.01
CLA	5 C4A	-13.759	-44.492	182.465
CLA	5 CMA	-13.072	-44.143	180.069
CLA	5 HMA1	-12.479	-44.526	179.231
CLA	5 HMA2	-12.697	-43.151	180.344
CLA	5 HMA3	-14.103	-44.034	179.739
CLA	5 CAA	-11.205	-46.679	182.166
CLA	5 HAA1	-11.954	-47.062	182.865
CLA	5 HAA2	-10.245	-46.724	182.683
CLA	5 CBA	-11.139	-47.583	180.929

CLA	5 HBA1	-10.303	-47.266	180.297
CLA	5 HBA2	-12.055	-47.536	180.339
CLA	5 CGA	-10.948	-49.026	181.328
CLA	5 O1A	-11.752	-49.91	181.133
CLA	5 O2A	-9.776	-49.191	181.963
CLA	5 NB	-15.471	-43.267	184.673
CLA	5 C1B	-15.946	-43.965	183.616
CLA	5 C2B	-17.403	-44.075	183.702
CLA	5 C3B	-17.779	-43.397	184.84
CLA	5 C4B	-16.546	-42.905	185.455
CLA	5 CMB	-18.281	-44.834	182.762
CLA	5 HMB1	-17.976	-45.885	182.688
CLA	5 HMB2	-18.267	-44.422	181.746
CLA	5 HMB3	-19.309	-44.804	183.123
CLA	5 CAB	-19.098	-43.177	185.447
CLA	5 HAB	-19.165	-43.425	186.505
CLA	5 CBB	-20.173	-42.641	184.857
CLA	5 HBB1	-21.089	-42.459	185.409
CLA	5 HBB2	-20.161	-42.309	183.826
CLA	5 NC	-14.069	-42.074	186.968
CLA	5 C1C	-15.33	-41.729	187.323
CLA	5 C2C	-15.312	-40.848	188.488
CLA	5 C3C	-13.991	-40.69	188.834
CLA	5 C4C	-13.224	-41.486	187.881
CLA	5 CMC	-16.514	-40.236	189.132
CLA	5 HMC1	-17.04	-40.967	189.756
CLA	5 HMC2	-17.218	-39.849	188.388
CLA	5 HMC3	-16.24	-39.404	189.785
CLA	5 CAC	-13.425	-39.785	189.89
CLA	5 HAC1	-12.97	-40.366	190.7
CLA	5 HAC2	-14.247	-39.233	190.353
CLA	5 CBC	-12.393	-38.781	189.333
CLA	5 HBC1	-11.375	-39.169	189.425
CLA	5 HBC2	-12.434	-37.838	189.877
CLA	5 HBC3	-12.592	-38.558	188.28
CLA	5 ND	-11.634	-42.85	185.754
CLA	5 C1D	-11.078	-42.362	186.923
CLA	5 C2D	-9.635	-42.611	186.937
CLA	5 C3D	-9.37	-43.21	185.722
CLA	5 C4D	-10.612	-43.352	185.049
CLA	5 CMD	-8.681	-42.296	188.024
CLA	5 HMD1	-8.639	-43.085	188.78
CLA	5 HMD2	-9.005	-41.392	188.524
CLA	5 HMD3	-7.67	-42.156	187.639
CLA	5 CAD	-8.31	-43.781	184.902
CLA	5 OBD	-7.118	-43.859	185.11
CLA	5 CBD	-9.036	-44.339	183.599
CLA	5 HBD1	-8.809	-45.404	183.502
CLA	5 CGD	-8.452	-43.606	182.415
CLA	5 O1D	-8.61	-42.418	182.251
CLA	5 O2D	-7.721	-44.39	181.624
CLA	5 CED	-6.936	-43.718	180.612
CLA	5 HED1	-6.674	-42.716	180.94
CLA	5 HED2	-7.498	-43.654	179.684

CLA	5	HED3	-6.047	-44.322	180.466
CLA	5	C1	-9.498	-50.523	182.417
CLA	5	H1	-9.685	-51.249	181.625
CLA	5	H2	-10.113	-50.754	183.287
CLA	5	H3	-8.446	-50.527	182.698

(d) Atomic coordinates in calculations with axial ligands in QM region.

(d-1) wild type.

residue			atom	x	y	z
HIS	A	198	ND1	-19.533	-48.497	191.835
HIS	A	198	HD1	-18.841	-49.141	192.244
HIS	A	198	CG	-20.912	-48.558	191.883
HIS	A	198	CB	-21.624	-49.595	192.695
HIS	A	198	HB1	-22.519	-49.164	193.152
HIS	A	198	HB2	-20.974	-49.968	193.49
HIS	A	198	NE2	-20.237	-46.896	190.516
HIS	A	198	CD2	-21.331	-47.541	191.061
HIS	A	198	HD2	-22.338	-47.228	190.835
HIS	A	198	CE1	-19.171	-47.51	191.001
HIS	A	198	HE1	-18.144	-47.272	190.773
HIS	D	197	ND1	-13.918	-38.655	184.061
HIS	D	197	HD1	-14.526	-37.827	184.136
HIS	D	197	CG	-12.828	-38.82	183.233
HIS	D	197	CB	-12.273	-37.689	182.416
HIS	D	197	HB1	-11.235	-37.493	182.663
HIS	D	197	HB2	-12.813	-36.768	182.649
HIS	D	197	NE2	-13.42	-40.792	184.156
HIS	D	197	CD2	-12.535	-40.16	183.307
HIS	D	197	HD2	-11.731	-40.703	182.832
HIS	D	197	CE1	-14.246	-39.849	184.585
HIS	D	197	HE1	-15.075	-39.988	185.26
CLA		4	MG	-19.976	-45.076	189.503
CLA		4	CHA	-23.392	-44.796	188.854
CLA		4	CHB	-19.605	-46.533	186.437
CLA		4	HHB	-19.478	-47.111	185.532
CLA		4	CHC	-16.587	-44.397	189.57
CLA		4	HHC	-15.519	-44.229	189.621
CLA		4	CHD	-20.387	-42.867	192.186
CLA		4	HHD	-20.51	-42.248	193.069
CLA		4	NA	-21.326	-45.515	187.845
CLA		4	C1A	-22.695	-45.341	187.806
CLA		4	C2A	-23.25	-45.753	186.458
CLA		4	H2A	-24.207	-46.274	186.565
CLA		4	C3A	-22.129	-46.686	185.952
CLA		4	H3A	-21.944	-46.559	184.88
CLA		4	C4A	-20.932	-46.213	186.773
CLA		4	CMA	-22.414	-48.165	186.256
CLA		4	HMA1	-23.306	-48.512	185.724
CLA		4	HMA2	-22.578	-48.313	187.329
CLA		4	HMA3	-21.568	-48.785	185.953
CLA		4	CAA	-23.445	-44.499	185.568
CLA		4	HAA1	-22.459	-44.094	185.321
CLA		4	HAA2	-23.975	-43.727	186.133
CLA		4	CBA	-24.212	-44.75	184.27
CLA		4	HBA1	-23.771	-45.554	183.671
CLA		4	HBA2	-24.173	-43.851	183.643
CLA		4	CGA	-25.675	-45.068	184.504
CLA		4	O1A	-26.262	-44.95	185.56
CLA		4	O2A	-26.26	-45.502	183.369

CLA	4 NB	-18.371	-45.401	188.229
CLA	4 C1B	-18.426	-46.134	187.069
CLA	4 C2B	-17.082	-46.381	186.565
CLA	4 C3B	-16.218	-45.724	187.417
CLA	4 C4B	-17.059	-45.14	188.471
CLA	4 CMB	-16.75	-47.219	185.377
CLA	4 HMB1	-17.593	-47.84	185.064
CLA	4 HMB2	-15.918	-47.887	185.615
CLA	4 HMB3	-16.448	-46.606	184.52
CLA	4 CAB	-14.777	-45.548	187.356
CLA	4 HAB	-14.32	-45.107	188.236
CLA	4 CBB	-13.961	-45.815	186.325
CLA	4 HBB1	-12.902	-45.596	186.393
CLA	4 HBB2	-14.321	-46.183	185.374
CLA	4 NC	-18.704	-43.891	190.711
CLA	4 C1C	-17.339	-43.798	190.578
CLA	4 C2C	-16.785	-42.946	191.621
CLA	4 C3C	-17.842	-42.522	192.382
CLA	4 C4C	-19.044	-43.123	191.785
CLA	4 CMC	-15.334	-42.62	191.797
CLA	4 HMC1	-14.884	-42.276	190.86
CLA	4 HMC2	-14.77	-43.487	192.139
CLA	4 HMC3	-15.184	-41.845	192.545
CLA	4 CAC	-17.74	-41.642	193.593
CLA	4 HAC1	-17.094	-42.161	194.313
CLA	4 HAC2	-18.718	-41.556	194.065
CLA	4 CBC	-17.169	-40.228	193.363
CLA	4 HBC1	-16.259	-40.236	192.76
CLA	4 HBC2	-16.916	-39.78	194.325
CLA	4 HBC3	-17.878	-39.567	192.861
CLA	4 ND	-21.508	-44.053	190.371
CLA	4 C1D	-21.542	-43.259	191.513
CLA	4 C2D	-22.94	-42.897	191.815
CLA	4 C3D	-23.682	-43.499	190.821
CLA	4 C4D	-22.77	-44.201	189.984
CLA	4 CMD	-23.413	-42.104	192.972
CLA	4 HMD1	-22.564	-41.857	193.602
CLA	4 HMD2	-24.134	-42.67	193.568
CLA	4 HMD3	-23.915	-41.179	192.67
CLA	4 CAD	-25.016	-43.543	190.225
CLA	4 OBD	-26.023	-42.949	190.542
CLA	4 CBD	-24.872	-44.446	188.92
CLA	4 HBD1	-25.215	-43.859	188.063
CLA	4 CGD	-25.875	-45.549	189.033
CLA	4 O1D	-25.676	-46.637	189.533
CLA	4 O2D	-27.055	-45.102	188.601
CLA	4 CED	-28.184	-45.945	188.838
CLA	4 HED1	-28.067	-46.47	189.785
CLA	4 HED2	-28.281	-46.674	188.029
CLA	4 HED3	-29.045	-45.276	188.869
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.745	-46.613	184.31
CLA	4 H2	-27.933	-46.294	182.553
CLA	4 H3	-28.249	-44.997	183.748

CLA	5 MG	-13.507	-42.745	185.002
CLA	5 CHA	-10.497	-44.091	183.832
CLA	5 CHB	-15.129	-44.553	182.569
CLA	5 HHB	-15.668	-45.003	181.741
CLA	5 CHC	-16.472	-42.172	186.592
CLA	5 HHC	-17.422	-41.881	187.024
CLA	5 CHD	-11.826	-41.697	187.863
CLA	5 HHD	-11.289	-41.272	188.705
CLA	5 NA	-12.868	-44.093	183.398
CLA	5 C1A	-11.59	-44.423	183.053
CLA	5 C2A	-11.545	-45.264	181.798
CLA	5 H2A	-10.807	-44.874	181.084
CLA	5 C3A	-12.982	-45.117	181.265
CLA	5 H3A	-13.365	-46.094	180.97
CLA	5 C4A	-13.742	-44.57	182.472
CLA	5 CMA	-13.069	-44.148	180.084
CLA	5 HMA1	-12.479	-44.503	179.231
CLA	5 HMA2	-12.7	-43.16	180.382
CLA	5 HMA3	-14.103	-44.037	179.765
CLA	5 CAA	-11.177	-46.717	182.127
CLA	5 HAA1	-11.911	-47.106	182.839
CLA	5 HAA2	-10.206	-46.763	182.624
CLA	5 CBA	-11.136	-47.616	180.886
CLA	5 HBA1	-10.308	-47.303	180.242
CLA	5 HBA2	-12.062	-47.567	180.312
CLA	5 CGA	-10.945	-49.051	181.297
CLA	5 O1A	-11.755	-49.937	181.134
CLA	5 O2A	-9.766	-49.208	181.921
CLA	5 NB	-15.461	-43.327	184.668
CLA	5 C1B	-15.938	-44.021	183.611
CLA	5 C2B	-17.398	-44.107	183.685
CLA	5 C3B	-17.772	-43.419	184.82
CLA	5 C4B	-16.537	-42.939	185.436
CLA	5 CMB	-18.284	-44.856	182.746
CLA	5 HMB1	-17.998	-45.912	182.677
CLA	5 HMB2	-18.263	-44.449	181.728
CLA	5 HMB3	-19.312	-44.805	183.106
CLA	5 CAB	-19.088	-43.185	185.431
CLA	5 HAB	-19.151	-43.427	186.491
CLA	5 CBB	-20.163	-42.642	184.849
CLA	5 HBB1	-21.07	-42.449	185.413
CLA	5 HBB2	-20.159	-42.313	183.818
CLA	5 NC	-14.057	-42.085	186.934
CLA	5 C1C	-15.317	-41.734	187.283
CLA	5 C2C	-15.301	-40.851	188.445
CLA	5 C3C	-13.979	-40.699	188.797
CLA	5 C4C	-13.212	-41.501	187.849
CLA	5 CMC	-16.505	-40.238	189.087
CLA	5 HMC1	-17.048	-40.977	189.686
CLA	5 HMC2	-17.198	-39.828	188.345
CLA	5 HMC3	-16.232	-39.425	189.763
CLA	5 CAC	-13.418	-39.805	189.867
CLA	5 HAC1	-12.963	-40.394	190.671
CLA	5 HAC2	-14.244	-39.263	190.335

CLA	5 CBC	-12.389	-38.79	189.331
CLA	5 HBC1	-11.37	-39.177	189.419
CLA	5 HBC2	-12.433	-37.855	189.888
CLA	5 HBC3	-12.585	-38.553	188.28
CLA	5 ND	-11.621	-42.945	185.774
CLA	5 C1D	-11.061	-42.405	186.919
CLA	5 C2D	-9.617	-42.623	186.923
CLA	5 C3D	-9.352	-43.24	185.715
CLA	5 C4D	-10.599	-43.428	185.063
CLA	5 CMD	-8.658	-42.272	187.994
CLA	5 HMD1	-8.616	-43.035	188.778
CLA	5 HMD2	-8.977	-41.349	188.462
CLA	5 HMD3	-7.649	-42.15	187.599
CLA	5 CAD	-8.289	-43.79	184.891
CLA	5 OBD	-7.093	-43.843	185.089
CLA	5 CBD	-9.013	-44.367	183.593
CLA	5 HBD1	-8.758	-45.425	183.491
CLA	5 CGD	-8.451	-43.616	182.411
CLA	5 O1D	-8.623	-42.428	182.253
CLA	5 O2D	-7.711	-44.387	181.611
CLA	5 CED	-6.932	-43.7	180.607
CLA	5 HED1	-6.702	-42.689	180.934
CLA	5 HED2	-7.484	-43.655	179.672
CLA	5 HED3	-6.025	-44.279	180.473
CLA	5 C1	-9.498	-50.523	182.417
CLA	5 H1	-9.672	-51.273	181.643
CLA	5 H2	-10.13	-50.732	183.282
CLA	5 H3	-8.45	-50.52	182.717

(d-2) D1-H198Q.

residue			atom	x	y	z
GLN	A	198	CB	-21.707	-49.48	192.462
GLN	A	198	HB1	-22.525	-49.198	193.127
GLN	A	198	HB2	-20.836	-49.688	193.09
GLN	A	198	CG	-21.493	-48.345	191.419
GLN	A	198	HG1	-21.786	-48.634	190.406
GLN	A	198	HG2	-22.155	-47.505	191.639
GLN	A	198	CD	-20.154	-47.69	191.229
GLN	A	198	OE1	-19.989	-46.954	190.231
GLN	A	198	NE2	-19.197	-47.825	192.139
GLN	A	198	HE21	-18.277	-47.476	191.899
GLN	A	198	HE22	-19.185	-48.608	192.782
HIS	D	197	ND1	-13.919	-38.656	184.058
HIS	D	197	HD1	-14.527	-37.828	184.135
HIS	D	197	CG	-12.828	-38.82	183.232
HIS	D	197	CB	-12.273	-37.689	182.416
HIS	D	197	HB1	-11.235	-37.492	182.662
HIS	D	197	HB2	-12.813	-36.767	182.649
HIS	D	197	NE2	-13.419	-40.794	184.153
HIS	D	197	CD2	-12.533	-40.159	183.306
HIS	D	197	HD2	-11.728	-40.701	182.832
HIS	D	197	CE1	-14.247	-39.851	184.581
HIS	D	197	HE1	-15.077	-39.992	185.254
CLA		4	MG	-19.945	-45.125	189.468
CLA		4	CHA	-23.391	-44.841	188.847
CLA		4	CHB	-19.61	-46.528	186.385
CLA		4	HHB	-19.486	-47.111	185.483
CLA		4	CHC	-16.59	-44.393	189.506
CLA		4	HHC	-15.522	-44.221	189.546
CLA		4	CHD	-20.375	-42.93	192.174
CLA		4	HHD	-20.496	-42.298	193.046
CLA		4	NA	-21.325	-45.542	187.824
CLA		4	C1A	-22.695	-45.369	187.791
CLA		4	C2A	-23.255	-45.759	186.438
CLA		4	H2A	-24.213	-46.277	186.54
CLA		4	C3A	-22.138	-46.69	185.922
CLA		4	H3A	-21.96	-46.563	184.848
CLA		4	C4A	-20.936	-46.22	186.736
CLA		4	CMA	-22.424	-48.169	186.229
CLA		4	HMA1	-23.317	-48.517	185.7
CLA		4	HMA2	-22.587	-48.312	187.303
CLA		4	HMA3	-21.577	-48.79	185.928
CLA		4	CAA	-23.448	-44.494	185.563
CLA		4	HAA1	-22.462	-44.085	185.322
CLA		4	HAA2	-23.978	-43.729	186.137
CLA		4	CBA	-24.217	-44.729	184.264
CLA		4	HBA1	-23.776	-45.526	183.653
CLA		4	HBA2	-24.18	-43.822	183.648
CLA		4	CGA	-25.679	-45.052	184.498
CLA		4	O1A	-26.269	-44.925	185.551
CLA		4	O2A	-26.261	-45.501	183.367
CLA		4	NB	-18.374	-45.36	188.145

CLA	4 C1B	-18.431	-46.117	187.005
CLA	4 C2B	-17.085	-46.385	186.512
CLA	4 C3B	-16.221	-45.728	187.361
CLA	4 C4B	-17.063	-45.12	188.4
CLA	4 CMB	-16.755	-47.248	185.345
CLA	4HMB1	-17.593	-47.889	185.061
CLA	4HMB2	-15.911	-47.895	185.592
CLA	4HMB3	-16.473	-46.655	184.468
CLA	4 CAB	-14.776	-45.581	187.319
CLA	4 HAB	-14.317	-45.18	188.217
CLA	4 CBB	-13.96	-45.825	186.283
CLA	4HBB1	-12.897	-45.632	186.363
CLA	4HBB2	-14.326	-46.15	185.318
CLA	4 NC	-18.701	-43.927	190.672
CLA	4 C1C	-17.336	-43.829	190.537
CLA	4 C2C	-16.779	-43.018	191.609
CLA	4 C3C	-17.837	-42.607	192.379
CLA	4 C4C	-19.037	-43.184	191.765
CLA	4 CMC	-15.329	-42.723	191.815
CLA	4HMC1	-15.044	-41.749	191.405
CLA	4HMC2	-14.708	-43.468	191.319
CLA	4HMC3	-15.076	-42.723	192.879
CLA	4 CAC	-17.744	-41.767	193.614
CLA	4HAC1	-17.146	-42.331	194.343
CLA	4HAC2	-18.736	-41.646	194.052
CLA	4 CBC	-17.104	-40.38	193.431
CLA	4HBC1	-16.12	-40.443	192.96
CLA	4HBC2	-16.966	-39.912	194.407
CLA	4HBC3	-17.725	-39.718	192.822
CLA	4 ND	-21.502	-44.162	190.391
CLA	4 C1D	-21.53	-43.334	191.511
CLA	4 C2D	-22.919	-42.936	191.8
CLA	4 C3D	-23.667	-43.537	190.809
CLA	4 C4D	-22.766	-44.272	189.988
CLA	4 CMD	-23.384	-42.121	192.947
CLA	4HMD1	-22.538	-41.873	193.581
CLA	4HMD2	-24.113	-42.674	193.547
CLA	4HMD3	-23.88	-41.197	192.633
CLA	4 CAD	-25	-43.562	190.212
CLA	4 OBD	-26.001	-42.96	190.533
CLA	4 CBD	-24.867	-44.467	188.907
CLA	4HBD1	-25.196	-43.875	188.048
CLA	4 CGD	-25.888	-45.554	189.022
CLA	4 O1D	-25.708	-46.643	189.527
CLA	4 O2D	-27.062	-45.092	188.59
CLA	4 CED	-28.203	-45.918	188.837
CLA	4HED1	-28.094	-46.431	189.791
CLA	4HED2	-28.305	-46.657	188.038
CLA	4HED3	-29.055	-45.238	188.857
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.743	-46.62	184.305
CLA	4 H2	-27.938	-46.285	182.55
CLA	4 H3	-28.247	-44.998	183.759
CLA	5MG	-13.505	-42.747	184.995

CLA	5 CHA	-10.496	-44.093	183.829
CLA	5 CHB	-15.127	-44.552	182.56
CLA	5 HHB	-15.666	-45.001	181.73
CLA	5 CHC	-16.471	-42.169	186.579
CLA	5 HHC	-17.421	-41.876	187.01
CLA	5 CHD	-11.827	-41.698	187.859
CLA	5 HHD	-11.29	-41.274	188.702
CLA	5 NA	-12.867	-44.093	183.391
CLA	5 C1A	-11.589	-44.424	183.048
CLA	5 C2A	-11.543	-45.266	181.794
CLA	5 H2A	-10.803	-44.877	181.082
CLA	5 C3A	-12.979	-45.117	181.258
CLA	5 H3A	-13.362	-46.094	180.962
CLA	5 C4A	-13.741	-44.57	182.464
CLA	5 CMA	-13.062	-44.148	180.077
CLA	5 HMA1	-12.47	-44.502	179.225
CLA	5 HMA2	-12.694	-43.16	180.378
CLA	5 HMA3	-14.096	-44.037	179.755
CLA	5 CAA	-11.178	-46.719	182.124
CLA	5 HAA1	-11.914	-47.108	182.834
CLA	5 HAA2	-10.208	-46.766	182.624
CLA	5 CBA	-11.135	-47.618	180.883
CLA	5 HBA1	-10.307	-47.305	180.24
CLA	5 HBA2	-12.06	-47.569	180.308
CLA	5 CGA	-10.945	-49.053	181.295
CLA	5 O1A	-11.757	-49.938	181.135
CLA	5 O2A	-9.765	-49.21	181.917
CLA	5 NB	-15.46	-43.326	184.658
CLA	5 C1B	-15.937	-44.019	183.6
CLA	5 C2B	-17.397	-44.101	183.672
CLA	5 C3B	-17.771	-43.411	184.805
CLA	5 C4B	-16.535	-42.935	185.423
CLA	5 CMB	-18.285	-44.849	182.734
CLA	5 HMB1	-18.002	-45.906	182.666
CLA	5 HMB2	-18.263	-44.443	181.715
CLA	5 HMB3	-19.313	-44.796	183.094
CLA	5 CAB	-19.087	-43.174	185.417
CLA	5 HAB	-19.148	-43.416	186.476
CLA	5 CBB	-20.163	-42.633	184.836
CLA	5 HBB1	-21.07	-42.443	185.4
CLA	5 HBB2	-20.162	-42.304	183.804
CLA	5 NC	-14.056	-42.085	186.925
CLA	5 C1C	-15.315	-41.731	187.272
CLA	5 C2C	-15.301	-40.849	188.434
CLA	5 C3C	-13.98	-40.699	188.789
CLA	5 C4C	-13.212	-41.502	187.843
CLA	5 CMC	-16.506	-40.241	189.077
CLA	5 HMC1	-17.052	-40.986	189.667
CLA	5 HMC2	-17.198	-39.826	188.336
CLA	5 HMC3	-16.236	-39.432	189.759
CLA	5 CAC	-13.42	-39.81	189.862
CLA	5 HAC1	-12.963	-40.403	190.662
CLA	5 HAC2	-14.245	-39.268	190.333
CLA	5 CBC	-12.39	-38.792	189.329

CLA	5 HBC1	-11.37	-39.177	189.419
CLA	5 HBC2	-12.437	-37.857	189.887
CLA	5 HBC3	-12.585	-38.554	188.278
CLA	5 ND	-11.621	-42.946	185.77
CLA	5 C1D	-11.061	-42.407	186.915
CLA	5 C2D	-9.617	-42.623	186.919
CLA	5 C3D	-9.351	-43.24	185.711
CLA	5 C4D	-10.598	-43.429	185.059
CLA	5 CMD	-8.658	-42.27	187.99
CLA	5 HMD1	-8.616	-43.033	188.775
CLA	5 HMD2	-8.977	-41.346	188.458
CLA	5 HMD3	-7.649	-42.149	187.596
CLA	5 CAD	-8.288	-43.789	184.887
CLA	5 OBD	-7.091	-43.84	185.084
CLA	5 CBD	-9.013	-44.369	183.59
CLA	5 HBD1	-8.757	-45.428	183.491
CLA	5 CGD	-8.451	-43.622	182.407
CLA	5 O1D	-8.629	-42.436	182.242
CLA	5 O2D	-7.708	-44.394	181.613
CLA	5 CED	-6.931	-43.711	180.604
CLA	5 HED1	-6.7	-42.7	180.926
CLA	5 HED2	-7.485	-43.67	179.67
CLA	5 HED3	-6.024	-44.292	180.471
CLA	5 C1	-9.498	-50.523	182.417
CLA	5 H1	-9.669	-51.274	181.645
CLA	5 H2	-10.132	-50.73	183.28
CLA	5 H3	-8.452	-50.52	182.72

(d-3) D1-H198A + H_2O.

residue			atom	x	y	z
HIS	D	197	ND1	-13.916	-38.649	184.067
HIS	D	197	HD1	-14.523	-37.82	184.141
HIS	D	197	CG	-12.829	-38.817	183.234
HIS	D	197	CB	-12.274	-37.688	182.416
HIS	D	197	HB1	-11.235	-37.492	182.663
HIS	D	197	HB2	-12.813	-36.766	182.649
HIS	D	197	NE2	-13.421	-40.788	184.162
HIS	D	197	CD2	-12.538	-40.157	183.309
HIS	D	197	HD2	-11.737	-40.703	182.832
HIS	D	197	CE1	-14.244	-39.841	184.593
HIS	D	197	HE1	-15.07	-39.979	185.271
CLA		4	MG	-19.957	-45.147	189.604
CLA		4	CHA	-23.378	-44.811	188.891
CLA		4	CHB	-19.598	-46.591	186.497
CLA		4	HHB	-19.471	-47.149	185.579
CLA		4	CHC	-16.585	-44.438	189.622
CLA		4	HHC	-15.517	-44.267	189.664
CLA		4	CHD	-20.375	-42.846	192.208
CLA		4	HHD	-20.5	-42.211	193.08
CLA		4	NA	-21.316	-45.594	187.922
CLA		4	C1A	-22.681	-45.389	187.863
CLA		4	C2A	-23.237	-45.797	186.513
CLA		4	H2A	-24.191	-46.322	186.623
CLA		4	C3A	-22.116	-46.724	185.999
CLA		4	H3A	-21.92	-46.573	184.931
CLA		4	C4A	-20.923	-46.276	186.838
CLA		4	CMA	-22.409	-48.207	186.263
CLA		4	HMA1	-23.297	-48.539	185.714
CLA		4	HMA2	-22.583	-48.382	187.33
CLA		4	HMA3	-21.559	-48.818	185.949
CLA		4	CAA	-23.444	-44.546	185.62
CLA		4	HAA1	-22.461	-44.128	185.379
CLA		4	HAA2	-23.986	-43.78	186.181
CLA		4	CBA	-24.2	-44.807	184.317
CLA		4	HBA1	-23.754	-45.619	183.73
CLA		4	HBA2	-24.152	-43.916	183.68
CLA		4	CGA	-25.667	-45.123	184.538
CLA		4	O1A	-26.255	-45.037	185.596
CLA		4	O2A	-26.254	-45.512	183.388
CLA		4	NB	-18.37	-45.482	188.308
CLA		4	C1B	-18.422	-46.187	187.131
CLA		4	C2B	-17.079	-46.396	186.605
CLA		4	C3B	-16.219	-45.739	187.46
CLA		4	C4B	-17.059	-45.192	188.534
CLA		4	CMB	-16.744	-47.199	185.396
CLA		4	HMB1	-17.587	-47.808	185.058
CLA		4	HMB2	-15.917	-47.879	185.619
CLA		4	HMB3	-16.432	-46.564	184.558
CLA		4	CAB	-14.783	-45.534	187.386
CLA		4	HAB	-14.33	-45.068	188.255
CLA		4	CBB	-13.963	-45.81	186.36

CLA	4 HBB1	-12.908	-45.568	186.422
CLA	4 HBB2	-14.315	-46.208	185.418
CLA	4 NC	-18.694	-43.905	190.759
CLA	4 C1C	-17.33	-43.821	190.624
CLA	4 C2C	-16.77	-42.948	191.646
CLA	4 C3C	-17.825	-42.502	192.399
CLA	4 C4C	-19.031	-43.112	191.815
CLA	4 CMC	-15.316	-42.633	191.815
CLA	4 HMC1	-14.828	-42.457	190.851
CLA	4 HMC2	-14.787	-43.444	192.319
CLA	4 HMC3	-15.163	-41.747	192.428
CLA	4 CAC	-17.717	-41.601	193.594
CLA	4 HAC1	-17.062	-42.103	194.317
CLA	4 HAC2	-18.691	-41.513	194.073
CLA	4 CBC	-17.159	-40.187	193.337
CLA	4 HBC1	-16.255	-40.195	192.724
CLA	4 HBC2	-16.896	-39.723	194.29
CLA	4 HBC3	-17.877	-39.537	192.834
CLA	4 ND	-21.495	-44.059	190.407
CLA	4 C1D	-21.53	-43.246	191.535
CLA	4 C2D	-22.929	-42.876	191.826
CLA	4 C3D	-23.668	-43.483	190.834
CLA	4 C4D	-22.757	-44.203	190.012
CLA	4 CMD	-23.411	-42.08	192.976
CLA	4 HMD1	-22.566	-41.839	193.612
CLA	4 HMD2	-24.14	-42.644	193.565
CLA	4 HMD3	-23.907	-41.154	192.671
CLA	4 CAD	-25.002	-43.533	190.237
CLA	4 OBD	-26.011	-42.943	190.554
CLA	4 CBD	-24.857	-44.445	188.94
CLA	4 HBD1	-25.186	-43.859	188.077
CLA	4 CGD	-25.872	-45.54	189.039
CLA	4 O1D	-25.682	-46.638	189.516
CLA	4 O2D	-27.05	-45.075	188.621
CLA	4 CED	-28.181	-45.924	188.836
CLA	4 HED1	-28.074	-46.458	189.779
CLA	4 HED2	-28.265	-46.645	188.019
CLA	4 HED3	-29.043	-45.257	188.863
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.757	-46.64	184.283
CLA	4 H2	-27.934	-46.254	182.537
CLA	4 H3	-28.239	-44.998	183.779
CLA	5 MG	-13.506	-42.743	185.003
CLA	5 CHA	-10.497	-44.09	183.833
CLA	5 CHB	-15.129	-44.546	182.567
CLA	5 HHB	-15.668	-44.995	181.738
CLA	5 CHC	-16.471	-42.188	186.603
CLA	5 HHC	-17.421	-41.903	187.039
CLA	5 CHD	-11.824	-41.693	187.862
CLA	5 HHD	-11.286	-41.267	188.703
CLA	5 NA	-12.868	-44.088	183.396
CLA	5 C1A	-11.59	-44.421	183.053
CLA	5 C2A	-11.545	-45.263	181.798
CLA	5 H2A	-10.806	-44.874	181.085

CLA	5 C3A	-12.982	-45.114	181.264
CLA	5 H3A	-13.366	-46.091	180.97
CLA	5 C4A	-13.742	-44.564	182.47
CLA	5 CMA	-13.066	-44.147	180.082
CLA	5HMA1	-12.476	-44.503	179.23
CLA	5HMA2	-12.697	-43.159	180.38
CLA	5HMA3	-14.1	-44.035	179.761
CLA	5 CAA	-11.18	-46.716	182.128
CLA	5HAA1	-11.916	-47.105	182.838
CLA	5HAA2	-10.21	-46.763	182.628
CLA	5 CBA	-11.136	-47.616	180.887
CLA	5HBA1	-10.308	-47.302	180.244
CLA	5HBA2	-12.061	-47.566	180.311
CLA	5 CGA	-10.946	-49.051	181.297
CLA	5 O1A	-11.756	-49.937	181.135
CLA	5 O2A	-9.766	-49.208	181.921
CLA	5 NB	-15.46	-43.328	184.671
CLA	5 C1B	-15.937	-44.019	183.612
CLA	5 C2B	-17.396	-44.111	183.689
CLA	5 C3B	-17.77	-43.432	184.829
CLA	5 C4B	-16.535	-42.95	185.444
CLA	5 CMB	-18.282	-44.86	182.748
CLA	5HMB1	-17.993	-45.915	182.677
CLA	5HMB2	-18.262	-44.45	181.732
CLA	5HMB3	-19.309	-44.814	183.109
CLA	5 CAB	-19.087	-43.21	185.442
CLA	5 HAB	-19.154	-43.469	186.498
CLA	5 CBB	-20.16	-42.66	184.863
CLA	5HBB1	-21.072	-42.479	185.422
CLA	5HBB2	-20.15	-42.316	183.836
CLA	5 NC	-14.055	-42.091	186.938
CLA	5 C1C	-15.315	-41.746	187.291
CLA	5 C2C	-15.3	-40.863	188.454
CLA	5 C3C	-13.978	-40.707	188.803
CLA	5 C4C	-13.21	-41.504	187.851
CLA	5 CMC	-16.504	-40.253	189.097
CLA	5HMC1	-17.038	-40.99	189.708
CLA	5HMC2	-17.205	-39.857	188.355
CLA	5HMC3	-16.233	-39.43	189.762
CLA	5 CAC	-13.419	-39.81	189.87
CLA	5HAC1	-12.963	-40.397	190.675
CLA	5HAC2	-14.245	-39.268	190.338
CLA	5 CBC	-12.391	-38.794	189.331
CLA	5HBC1	-11.371	-39.178	189.419
CLA	5HBC2	-12.436	-37.858	189.886
CLA	5HBC3	-12.588	-38.559	188.28
CLA	5 ND	-11.62	-42.942	185.774
CLA	5 C1D	-11.059	-42.402	186.917
CLA	5 C2D	-9.615	-42.62	186.921
CLA	5 C3D	-9.35	-43.237	185.713
CLA	5 C4D	-10.598	-43.426	185.062
CLA	5 CMD	-8.656	-42.27	187.993
CLA	5HMD1	-8.614	-43.033	188.776
CLA	5HMD2	-8.975	-41.346	188.462

CLA	5	HMD3	-7.647	-42.148	187.599
CLA	5	CAD	-8.288	-43.788	184.889
CLA	5	OBD	-7.092	-43.84	185.086
CLA	5	CBD	-9.014	-44.369	183.593
CLA	5	HBD1	-8.758	-45.427	183.494
CLA	5	CGD	-8.451	-43.622	182.41
CLA	5	O1D	-8.626	-42.436	182.246
CLA	5	O2D	-7.708	-44.395	181.615
CLA	5	CED	-6.931	-43.713	180.607
CLA	5	HED1	-6.699	-42.701	180.929
CLA	5	HED2	-7.484	-43.671	179.673
CLA	5	HED3	-6.024	-44.294	180.474
CLA	5	C1	-9.498	-50.523	182.417
CLA	5	H1	-9.67	-51.273	181.643
CLA	5	H2	-10.131	-50.732	183.281
CLA	5	H3	-8.451	-50.52	182.718
HOH	86	O	-17.057	-49.868	192.434
HOH	86	H1	-16.727	-50.587	191.86
HOH	86	H2	-16.961	-50.163	193.362
HOH	1	O	-20.461	-46.678	190.826
HOH	1	H1	-20.948	-46.398	191.615
HOH	1	H2	-19.835	-47.433	191.073
HOH	2	O	-18.92	-48.648	191.106
HOH	2	H1	-18.259	-49.03	191.741
HOH	2	H2	-19.361	-49.408	190.691

(d-4) D1-H198A – H_2O.

residue			atom	x	y	z
HIS	D	197	ND1	-13.919	-38.651	184.058
HIS	D	197	HD1	-14.528	-37.823	184.131
HIS	D	197	CG	-12.827	-38.817	183.233
HIS	D	197	CB	-12.272	-37.688	182.414
HIS	D	197	HB1	-11.234	-37.492	182.661
HIS	D	197	HB2	-12.811	-36.765	182.646
HIS	D	197	NE2	-13.421	-40.789	184.157
HIS	D	197	CD2	-12.534	-40.156	183.309
HIS	D	197	HD2	-11.729	-40.7	182.836
HIS	D	197	CE1	-14.249	-39.844	184.582
HIS	D	197	HE1	-15.081	-39.984	185.253
CLA		4	MG	-19.91	-44.936	189.386
CLA		4	CHA	-23.36	-44.876	188.887
CLA		4	CHB	-19.585	-46.573	186.413
CLA		4	HHB	-19.46	-47.127	185.493
CLA		4	CHC	-16.543	-44.449	189.537
CLA		4	HHC	-15.475	-44.282	189.577
CLA		4	CHD	-20.326	-42.932	192.184
CLA		4	HHD	-20.45	-42.288	193.048
CLA		4	NA	-21.293	-45.621	187.886
CLA		4	C1A	-22.662	-45.431	187.844
CLA		4	C2A	-23.223	-45.822	186.492
CLA		4	H2A	-24.177	-46.347	186.601
CLA		4	C3A	-22.106	-46.744	185.965
CLA		4	H3A	-21.931	-46.601	184.893
CLA		4	C4A	-20.901	-46.286	186.778
CLA		4	CMA	-22.387	-48.227	186.25
CLA		4	HMA1	-23.284	-48.568	185.723
CLA		4	HMA2	-22.538	-48.393	187.322
CLA		4	HMA3	-21.54	-48.835	185.927
CLA		4	CAA	-23.433	-44.562	185.612
CLA		4	HAA1	-22.452	-44.141	185.369
CLA		4	HAA2	-23.975	-43.801	186.18
CLA		4	CBA	-24.195	-44.815	184.309
CLA		4	HBA1	-23.754	-45.623	183.715
CLA		4	HBA2	-24.147	-43.919	183.678
CLA		4	CGA	-25.663	-45.126	184.533
CLA		4	O1A	-26.246	-45.038	185.594
CLA		4	O2A	-26.254	-45.513	183.385
CLA		4	NB	-18.34	-45.464	188.213
CLA		4	C1B	-18.4	-46.175	187.046
CLA		4	C2B	-17.063	-46.407	186.53
CLA		4	C3B	-16.192	-45.763	187.387
CLA		4	C4B	-17.016	-45.194	188.452
CLA		4	CMB	-16.74	-47.237	185.338
CLA		4	HMB1	-17.582	-47.863	185.033
CLA		4	HMB2	-15.903	-47.9	185.569
CLA		4	HMB3	-16.45	-46.621	184.477
CLA		4	CAB	-14.75	-45.597	187.317
CLA		4	HAB	-14.279	-45.201	188.21
CLA		4	CBB	-13.951	-45.829	186.264

CLA	4 HBB1	-12.888	-45.631	186.328
CLA	4 HBB2	-14.329	-46.155	185.304
CLA	4 NC	-18.65	-43.944	190.692
CLA	4 C1C	-17.287	-43.847	190.556
CLA	4 C2C	-16.733	-42.994	191.592
CLA	4 C3C	-17.791	-42.579	192.366
CLA	4 C4C	-18.99	-43.179	191.779
CLA	4 CMC	-15.28	-42.675	191.763
CLA	4 HMC1	-14.751	-42.693	190.807
CLA	4 HMC2	-14.792	-43.379	192.44
CLA	4 HMC3	-15.132	-41.687	192.197
CLA	4 CAC	-17.707	-41.725	193.596
CLA	4 HAC1	-17.076	-42.261	194.317
CLA	4 HAC2	-18.695	-41.648	194.052
CLA	4 CBC	-17.141	-40.302	193.417
CLA	4 HBC1	-16.192	-40.286	192.878
CLA	4 HBC2	-16.955	-39.867	194.401
CLA	4 HBC3	-17.829	-39.645	192.881
CLA	4 ND	-21.466	-44.202	190.428
CLA	4 C1D	-21.486	-43.356	191.537
CLA	4 C2D	-22.872	-42.95	191.819
CLA	4 C3D	-23.625	-43.551	190.831
CLA	4 C4D	-22.736	-44.306	190.021
CLA	4 CMD	-23.34	-42.136	192.966
CLA	4 HMD1	-22.493	-41.87	193.594
CLA	4 HMD2	-24.05	-42.703	193.575
CLA	4 HMD3	-23.86	-41.225	192.652
CLA	4 CAD	-24.958	-43.566	190.229
CLA	4 OBD	-25.952	-42.949	190.541
CLA	4 CBD	-24.832	-44.481	188.932
CLA	4 HBD1	-25.145	-43.888	188.068
CLA	4 CGD	-25.874	-45.553	189.035
CLA	4 O1D	-25.711	-46.651	189.519
CLA	4 O2D	-27.042	-45.065	188.612
CLA	4 CED	-28.189	-45.895	188.825
CLA	4 HED1	-28.096	-46.43	189.769
CLA	4 HED2	-28.28	-46.617	188.009
CLA	4 HED3	-29.04	-45.214	188.846
CLA	4 C1	-27.644	-45.876	183.518
CLA	4 H1	-27.751	-46.666	184.257
CLA	4 H2	-27.942	-46.218	182.527
CLA	4 H3	-28.234	-45.006	183.816
CLA	5 MG	-13.51	-42.742	184.993
CLA	5 CHA	-10.498	-44.098	183.833
CLA	5 CHB	-15.128	-44.544	182.556
CLA	5 HHB	-15.668	-44.992	181.728
CLA	5 CHC	-16.474	-42.181	186.586
CLA	5 HHC	-17.424	-41.892	187.02
CLA	5 CHD	-11.832	-41.703	187.859
CLA	5 HHD	-11.293	-41.282	188.701
CLA	5 NA	-12.868	-44.084	183.388
CLA	5 C1A	-11.596	-44.424	183.049
CLA	5 C2A	-11.547	-45.266	181.795
CLA	5 H2A	-10.804	-44.876	181.088

CLA	5 C3A	-12.981	-45.115	181.256
CLA	5 H3A	-13.366	-46.092	180.965
CLA	5 C4A	-13.744	-44.562	182.458
CLA	5 CMA	-13.059	-44.151	180.071
CLA	5 HMA1	-12.464	-44.511	179.224
CLA	5 HMA2	-12.692	-43.162	180.367
CLA	5 HMA3	-14.091	-44.042	179.742
CLA	5 CAA	-11.183	-46.72	182.126
CLA	5 HAA1	-11.92	-47.108	182.835
CLA	5 HAA2	-10.213	-46.768	182.626
CLA	5 CBA	-11.139	-47.617	180.885
CLA	5 HBA1	-10.311	-47.303	180.242
CLA	5 HBA2	-12.064	-47.569	180.309
CLA	5 CGA	-10.947	-49.053	181.296
CLA	5 O1A	-11.758	-49.937	181.134
CLA	5 O2A	-9.767	-49.208	181.919
CLA	5 NB	-15.461	-43.328	184.66
CLA	5 C1B	-15.937	-44.017	183.602
CLA	5 C2B	-17.398	-44.107	183.676
CLA	5 C3B	-17.773	-43.425	184.811
CLA	5 C4B	-16.537	-42.944	185.43
CLA	5 CMB	-18.282	-44.855	182.733
CLA	5 HMB1	-17.997	-45.911	182.667
CLA	5 HMB2	-18.256	-44.448	181.716
CLA	5 HMB3	-19.31	-44.804	183.09
CLA	5 CAB	-19.091	-43.198	185.421
CLA	5 HAB	-19.157	-43.459	186.476
CLA	5 CBB	-20.163	-42.645	184.843
CLA	5 HBB1	-21.075	-42.465	185.402
CLA	5 HBB2	-20.155	-42.3	183.817
CLA	5 NC	-14.06	-42.089	186.926
CLA	5 C1C	-15.317	-41.742	187.278
CLA	5 C2C	-15.303	-40.862	188.447
CLA	5 C3C	-13.984	-40.709	188.799
CLA	5 C4C	-13.215	-41.508	187.846
CLA	5 CMC	-16.508	-40.258	189.093
CLA	5 HMC1	-17.037	-41.001	189.701
CLA	5 HMC2	-17.209	-39.858	188.353
CLA	5 HMC3	-16.237	-39.439	189.762
CLA	5 CAC	-13.423	-39.818	189.869
CLA	5 HAC1	-12.967	-40.409	190.671
CLA	5 HAC2	-14.249	-39.277	190.339
CLA	5 CBC	-12.394	-38.801	189.332
CLA	5 HBC1	-11.373	-39.181	189.426
CLA	5 HBC2	-12.445	-37.863	189.884
CLA	5 HBC3	-12.588	-38.567	188.279
CLA	5 ND	-11.627	-42.948	185.769
CLA	5 C1D	-11.069	-42.411	186.91
CLA	5 C2D	-9.619	-42.629	186.917
CLA	5 C3D	-9.354	-43.244	185.712
CLA	5 C4D	-10.602	-43.434	185.058
CLA	5 CMD	-8.664	-42.274	187.99
CLA	5 HMD1	-8.625	-43.036	188.776
CLA	5 HMD2	-8.983	-41.349	188.456

CLA	5 HMD3	-7.653	-42.155	187.599
CLA	5 CAD	-8.291	-43.797	184.887
CLA	5 OBD	-7.096	-43.849	185.087
CLA	5 CBD	-9.016	-44.377	183.592
CLA	5 HBD1	-8.761	-45.436	183.491
CLA	5 CGD	-8.457	-43.625	182.408
CLA	5 O1D	-8.653	-42.443	182.241
CLA	5 O2D	-7.699	-44.387	181.62
CLA	5 CED	-6.933	-43.694	180.608
CLA	5 HED1	-6.72	-42.677	180.927
CLA	5 HED2	-7.488	-43.666	179.674
CLA	5 HED3	-6.016	-44.258	180.478
CLA	5 C1	-9.498	-50.523	182.417
CLA	5 H1	-9.672	-51.273	181.643
CLA	5 H2	-10.129	-50.73	183.282
CLA	5 H3	-8.45	-50.52	182.716